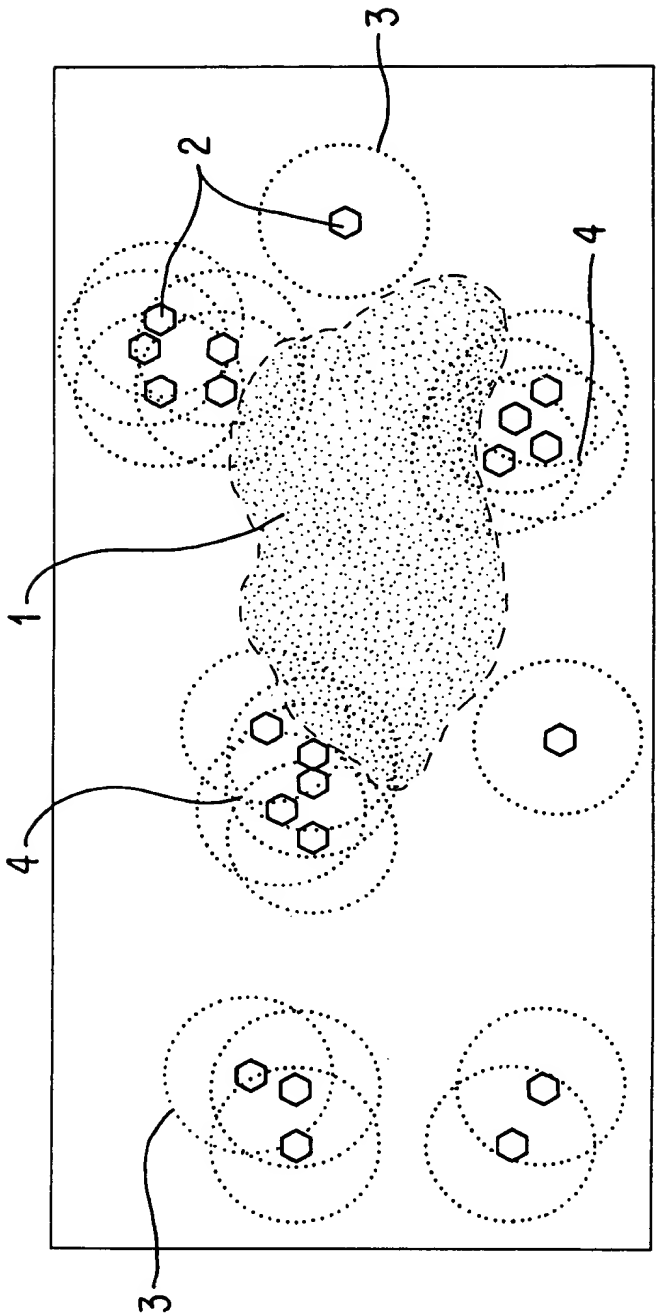


FIG. 1(a)

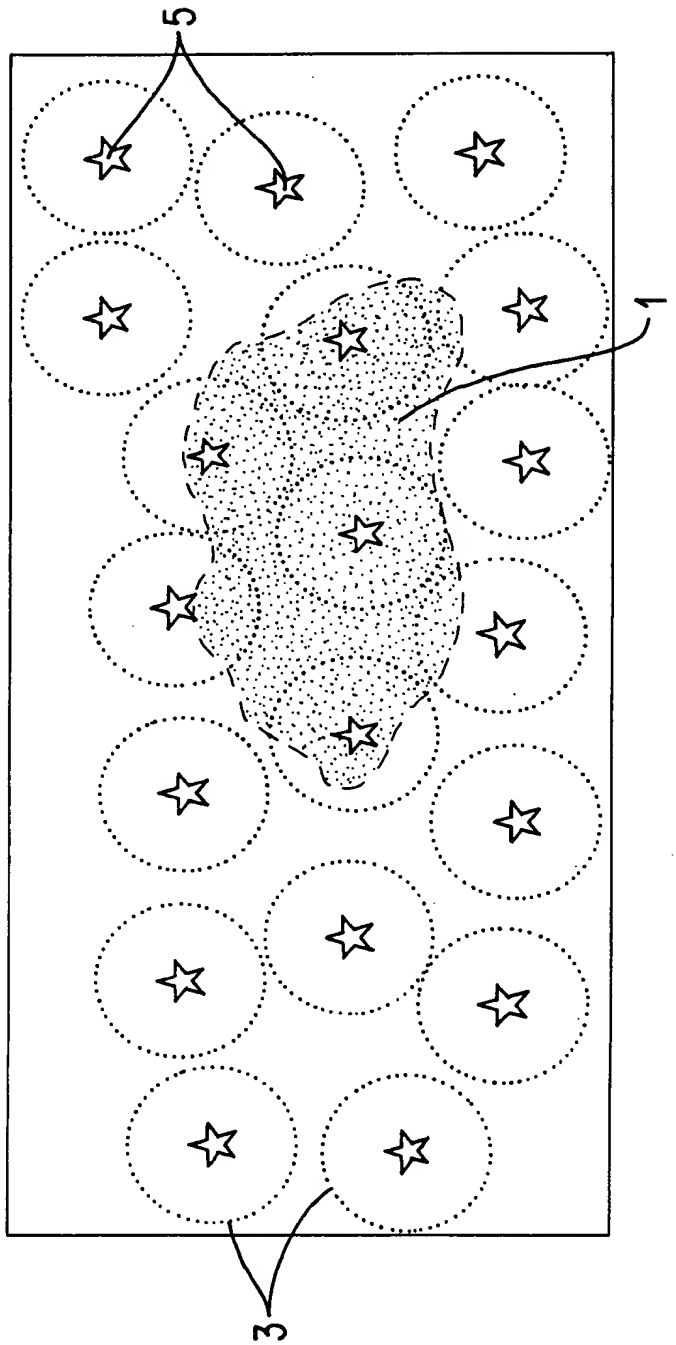


FIG.1(b)

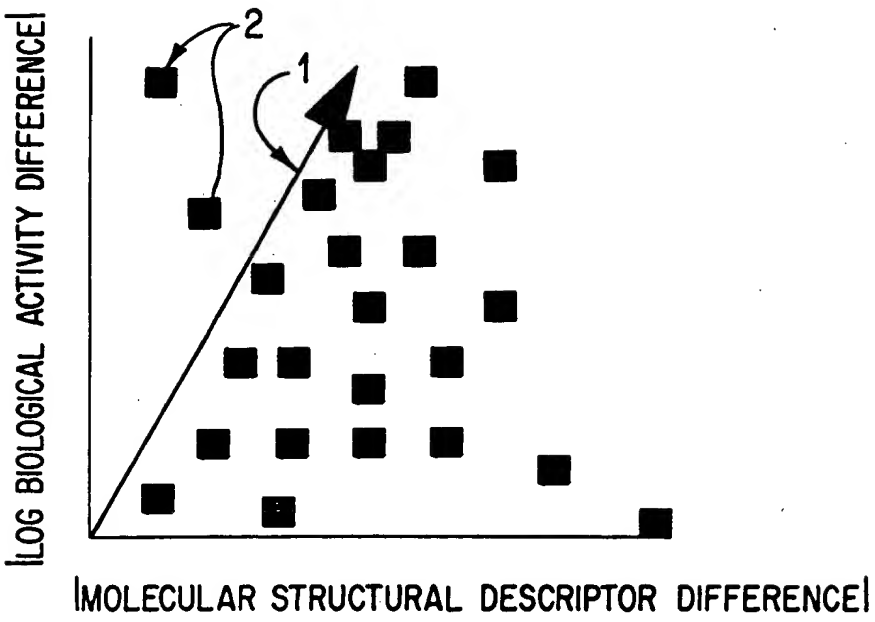


FIG. 2

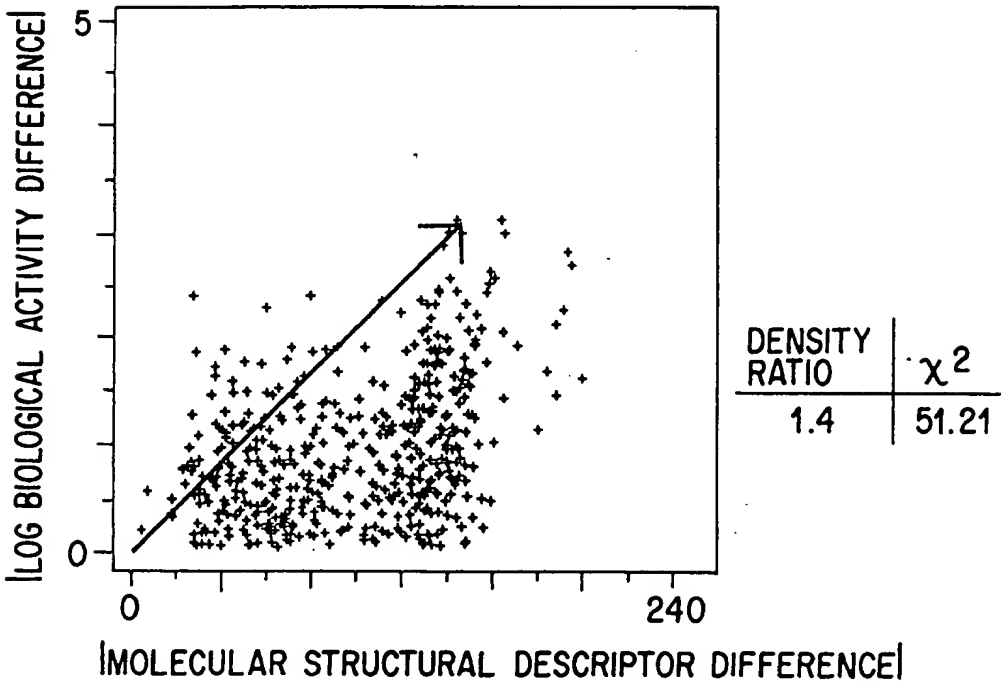
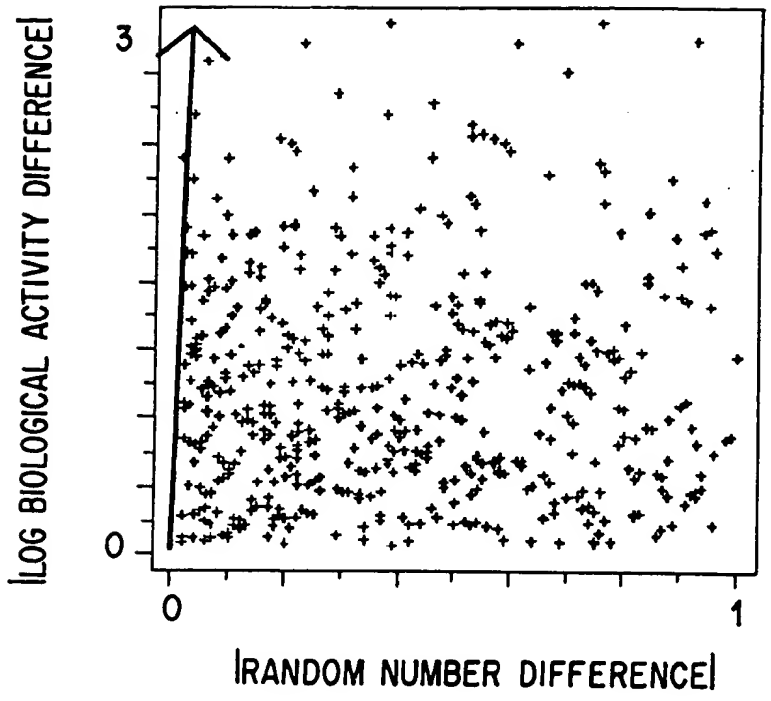
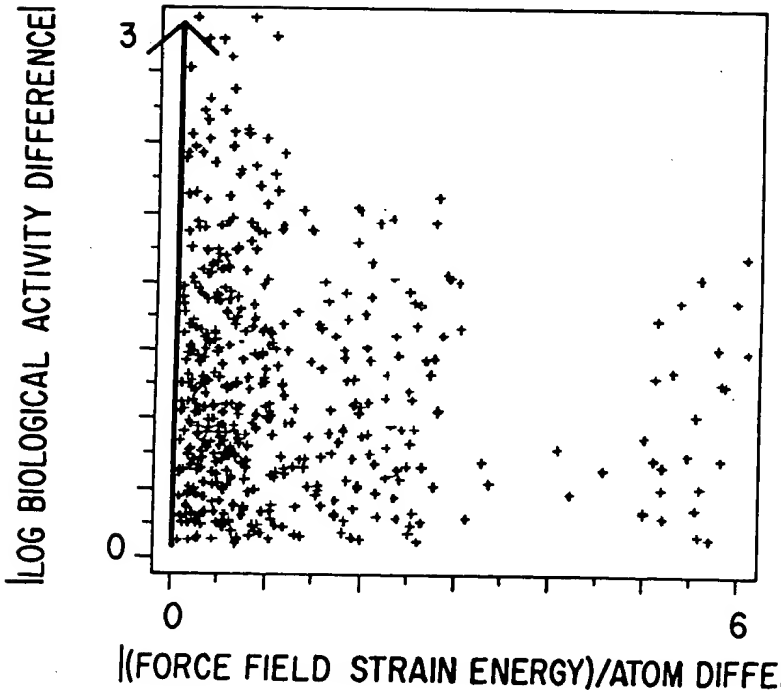


FIG. 3



DENSITY RATIO	χ^2
1.00	0.00

FIG. 4



DENSITY RATIO	χ^2
0.96	0.46

FIG. 5

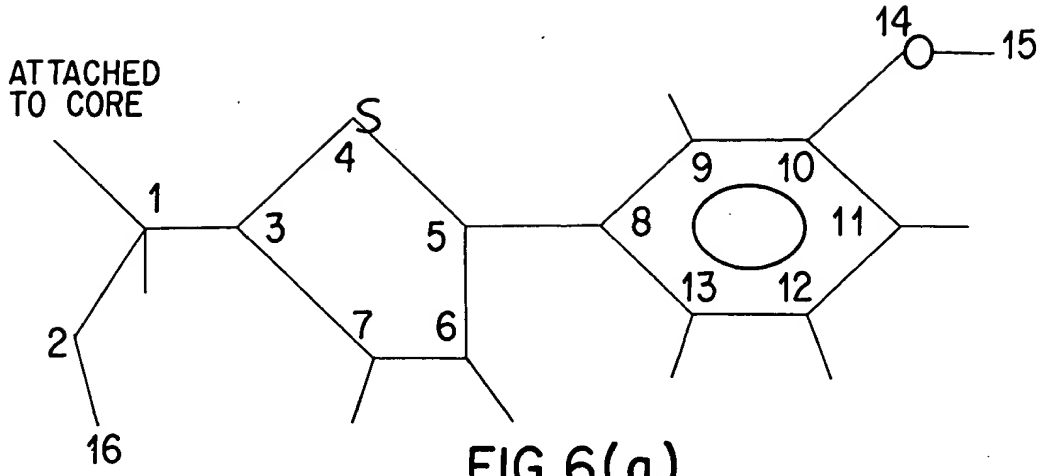


FIG. 6(a)

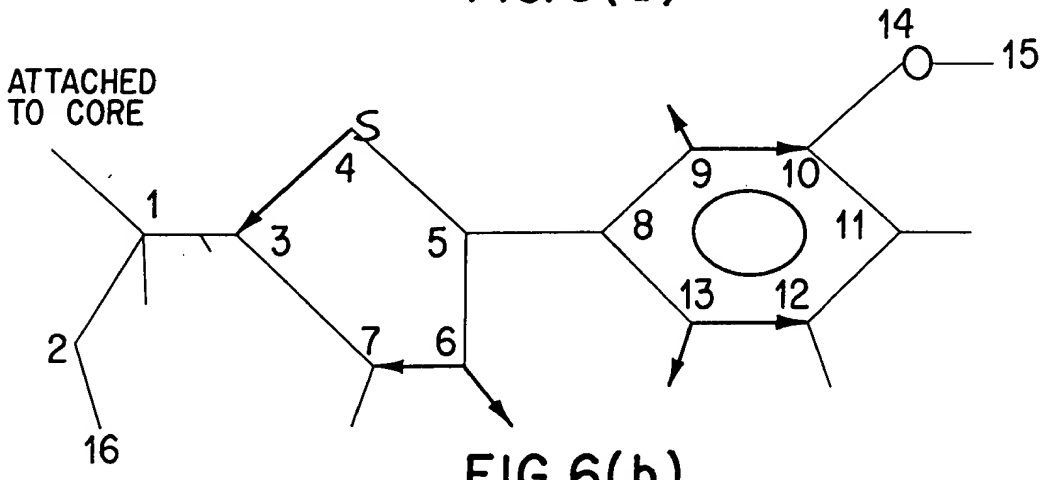


FIG. 6(b)

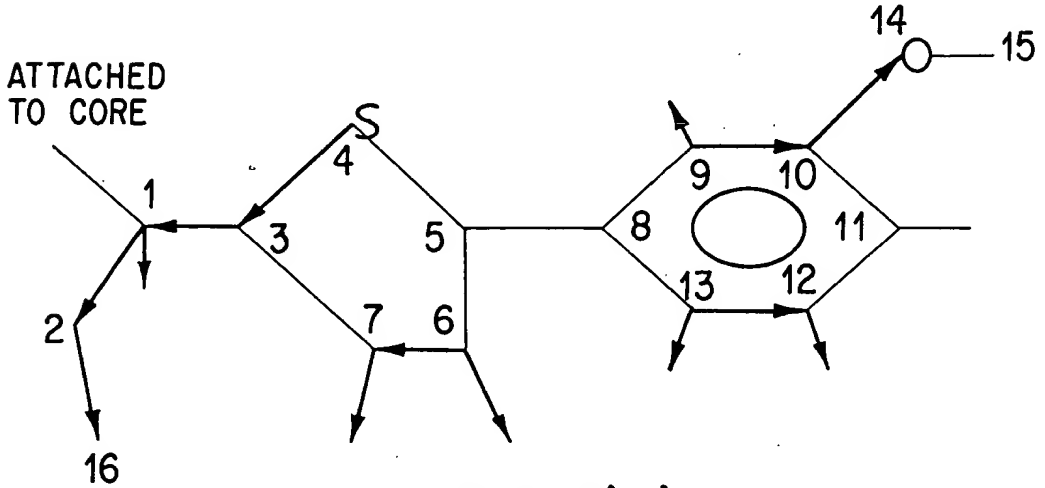


FIG. 6(c)

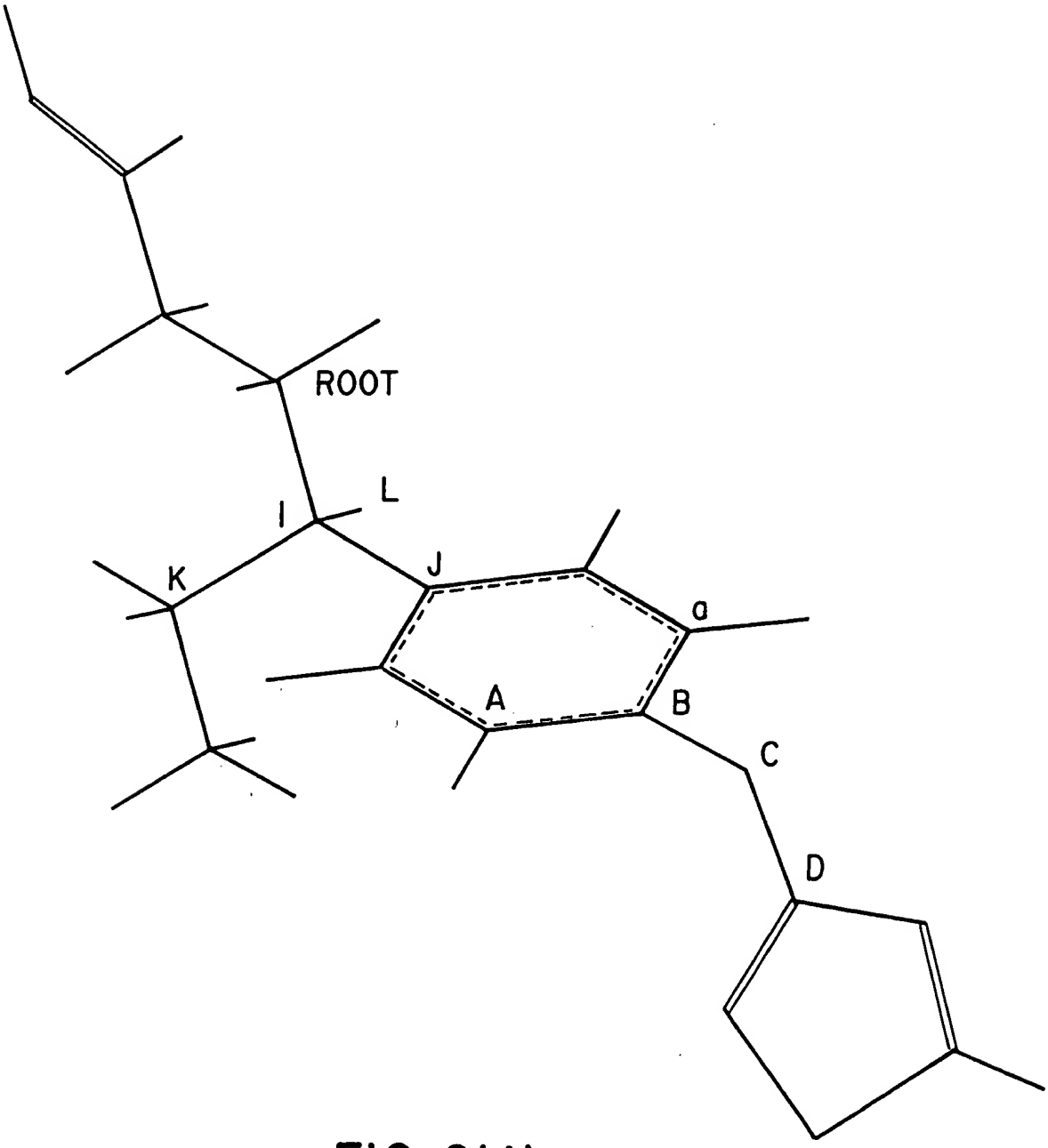


FIG. 6(d)

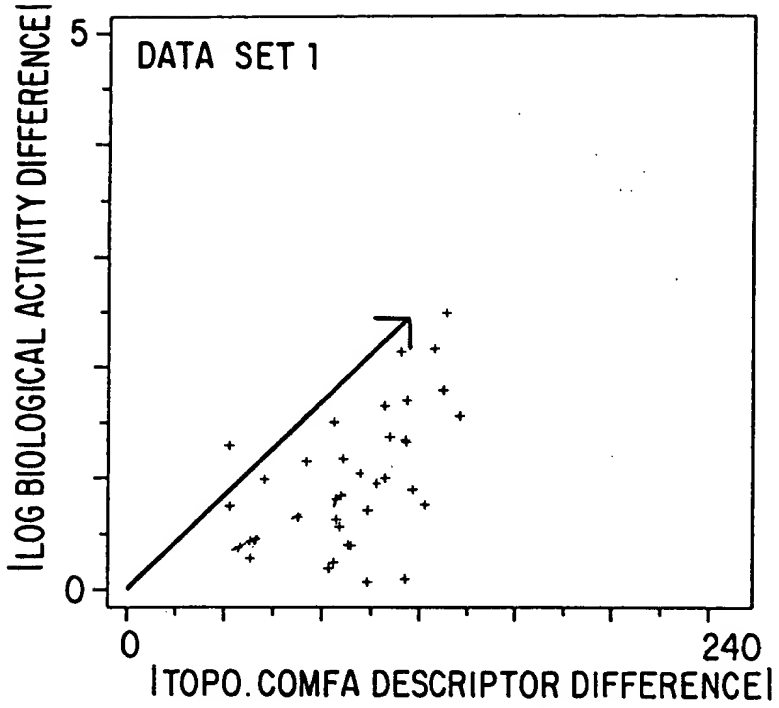

DATA SET 1
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
5
0
0
240
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG.7(a)

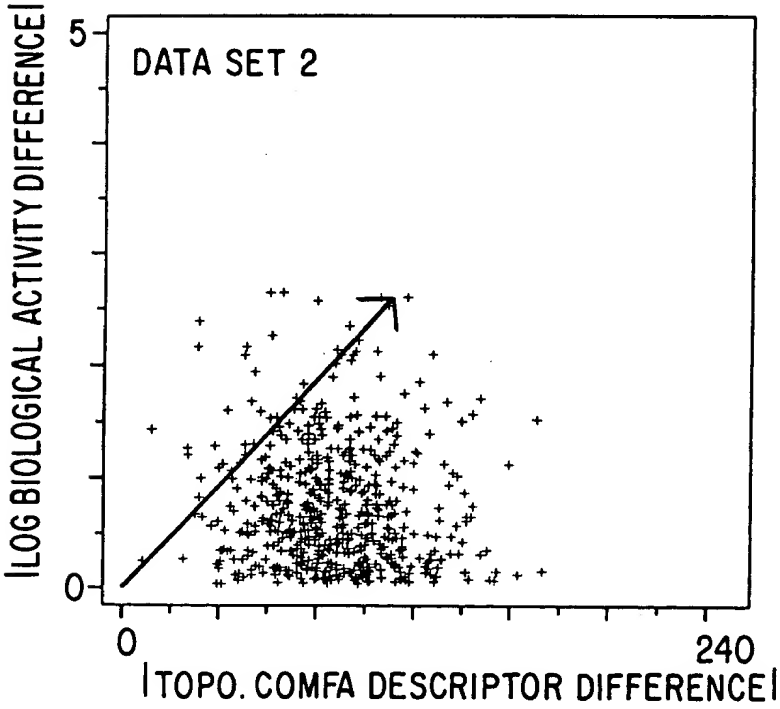

DATA SET 2
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
5
0
0
240
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG.7(b)

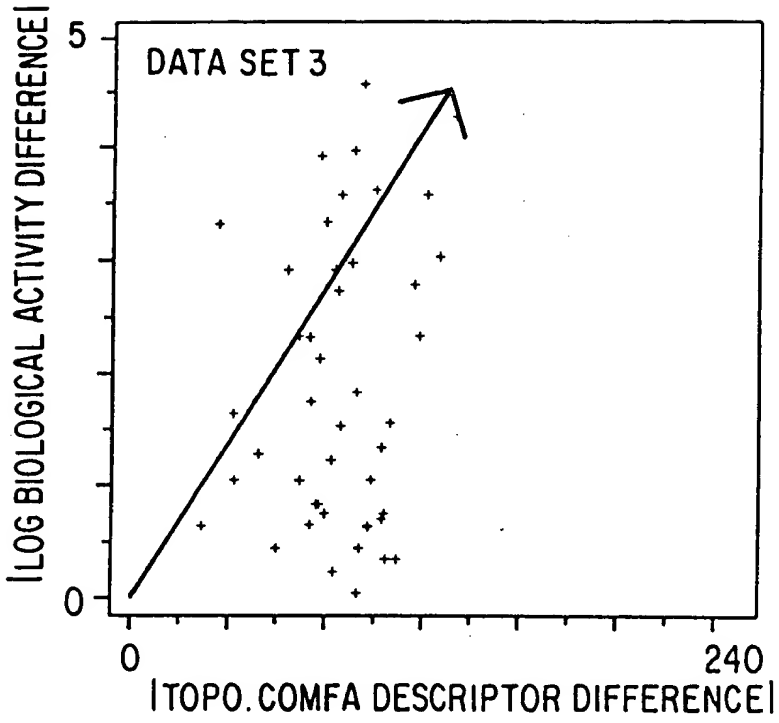


FIG. 7(c)

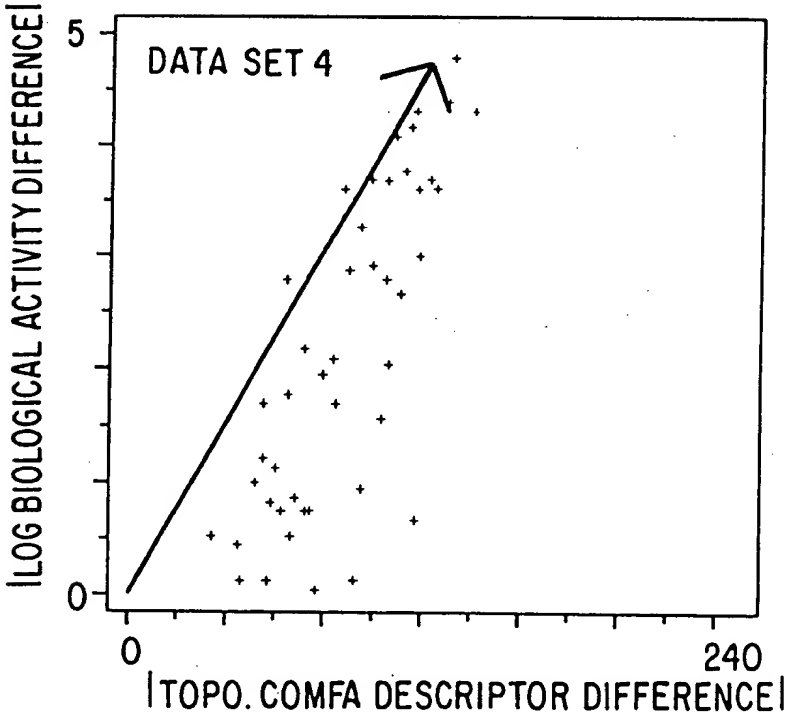


FIG. 7(d)

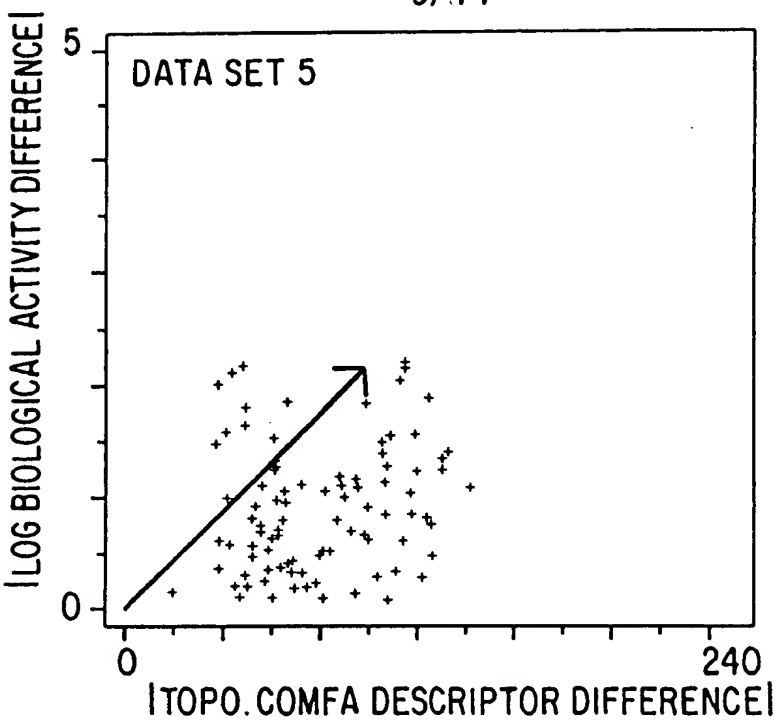


FIG. 7(e)

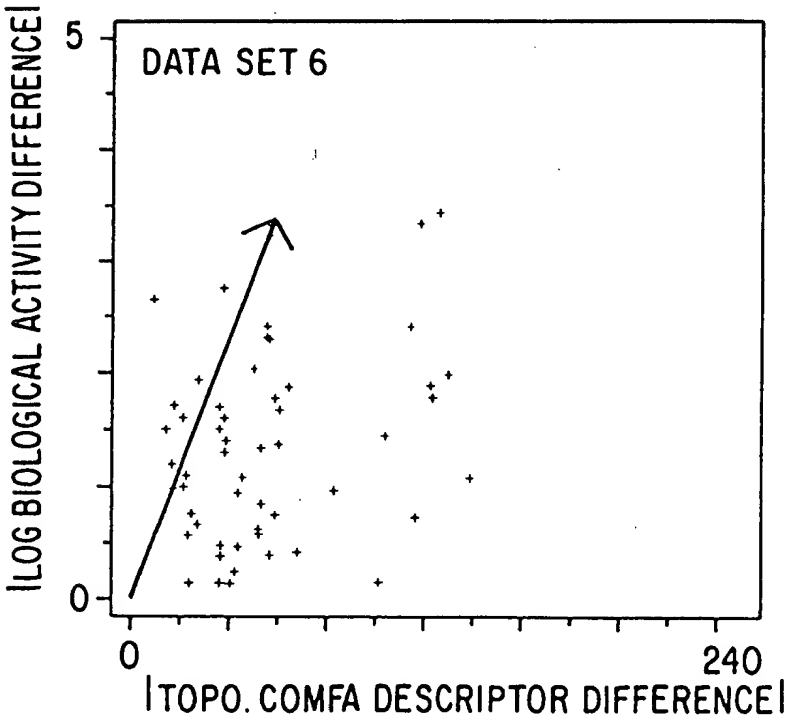


FIG. 7(f)

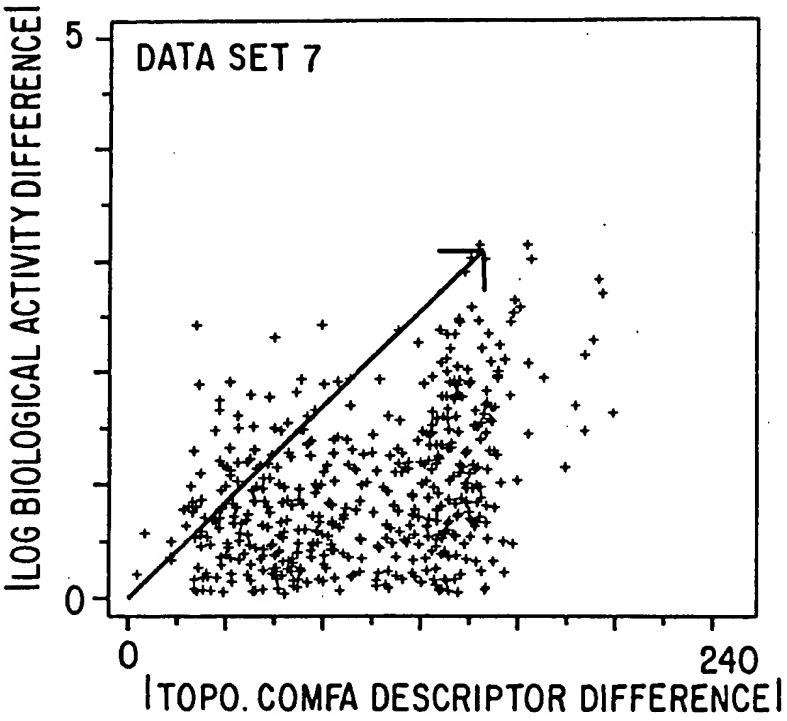


FIG.7(g)

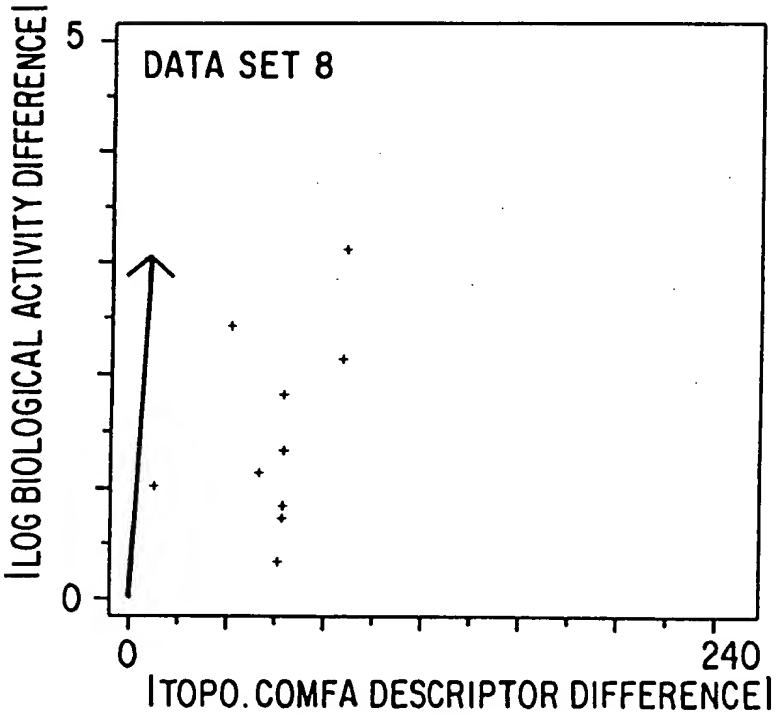


FIG.7(h)

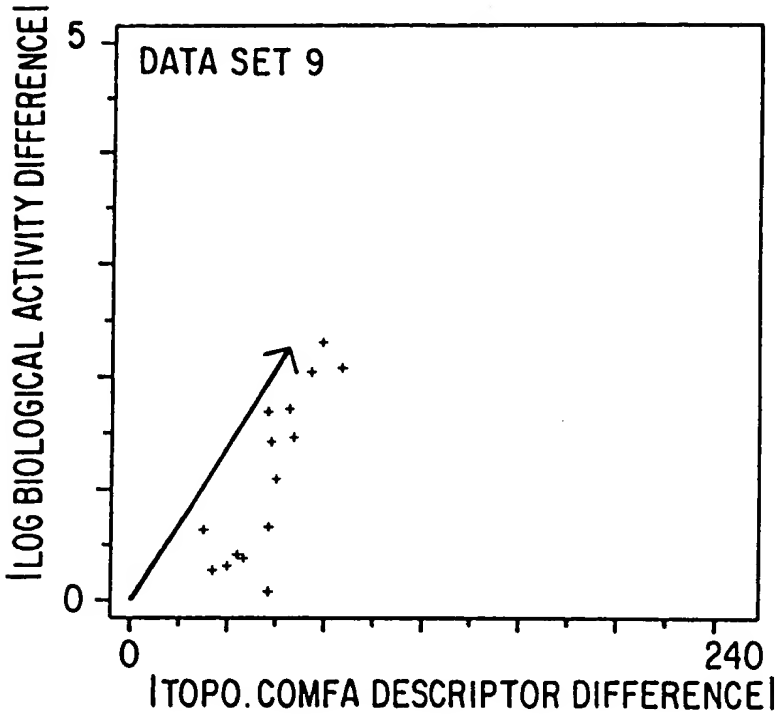


FIG. 7(i)

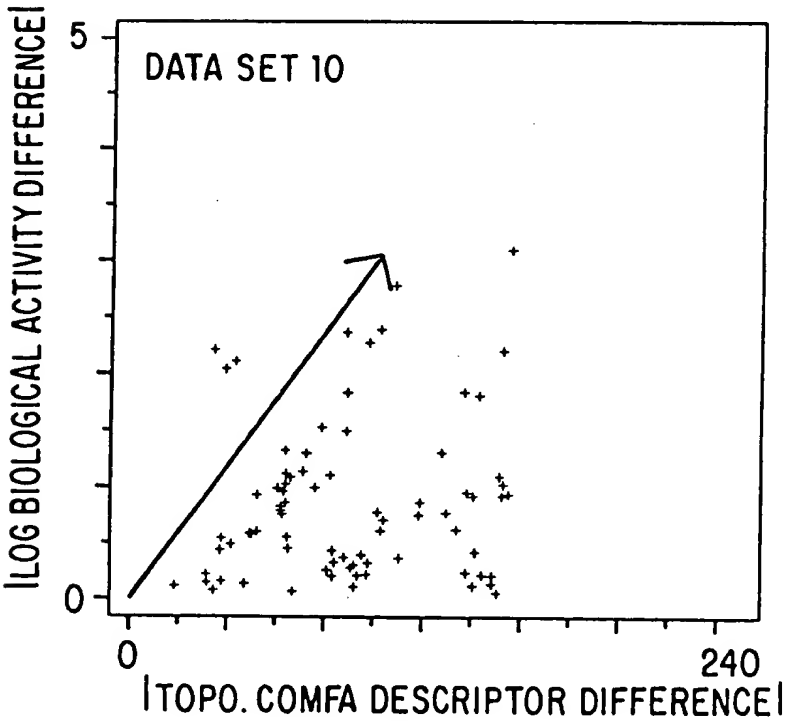


FIG. 7(j)

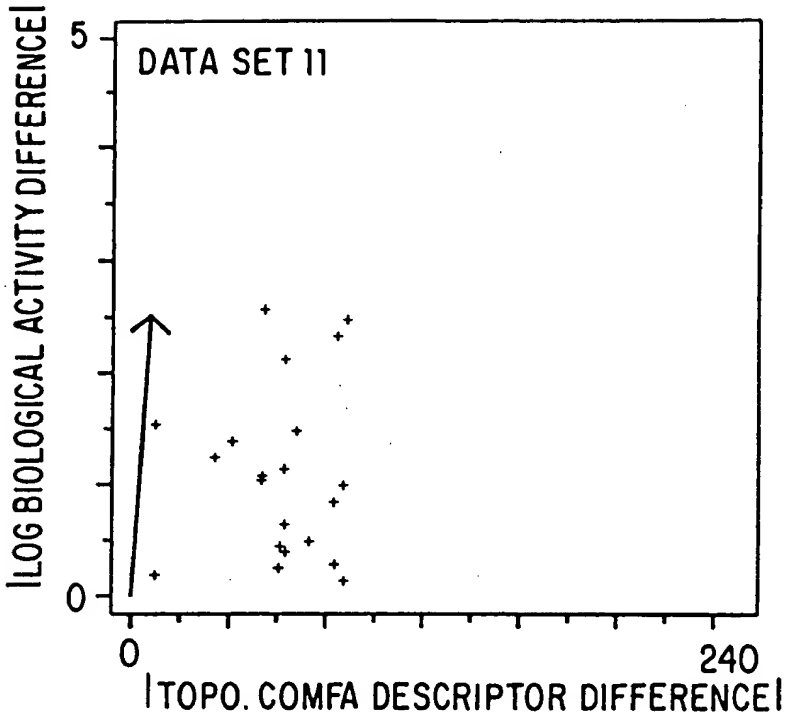


FIG.7(k)

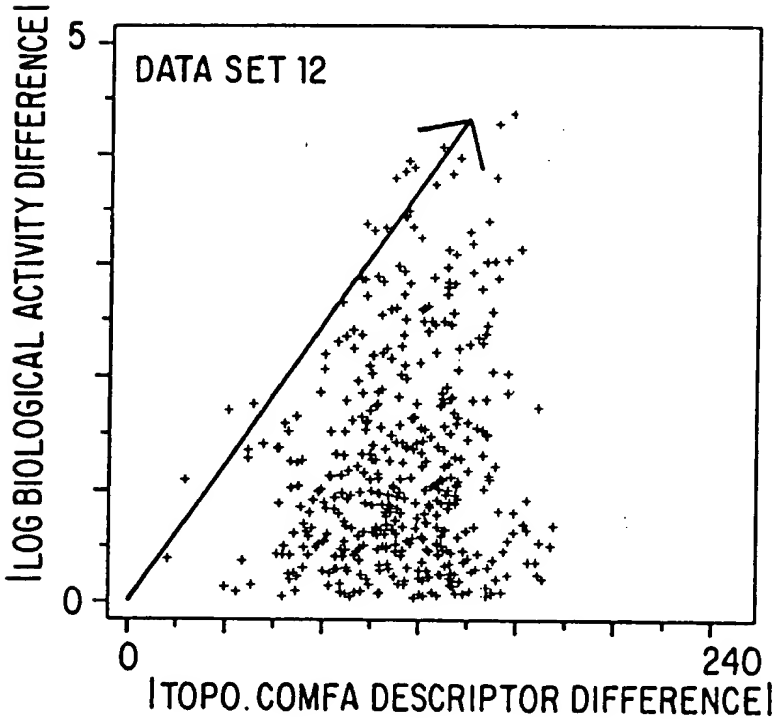


FIG.7(l)

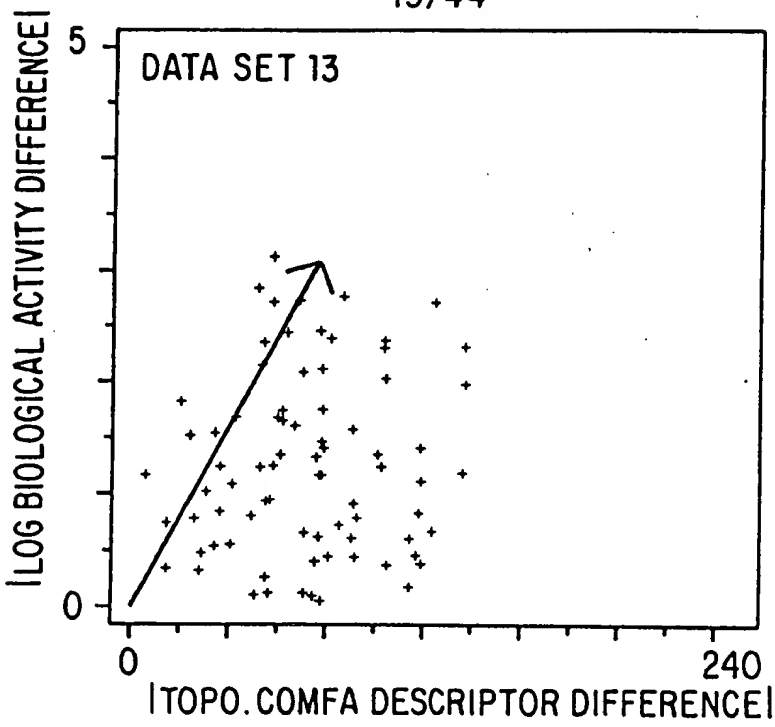


FIG. 7(m)

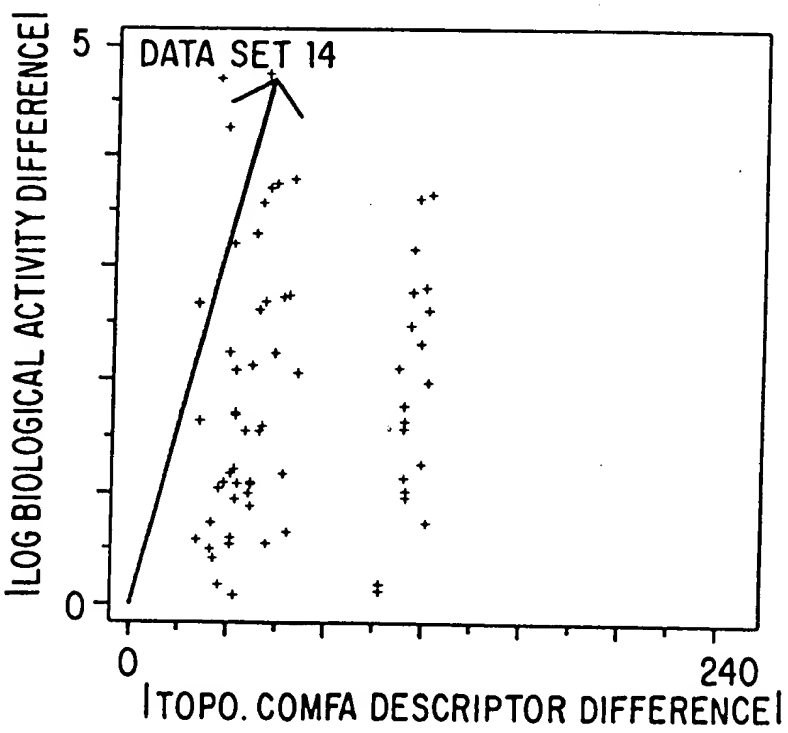


FIG. 7(n)

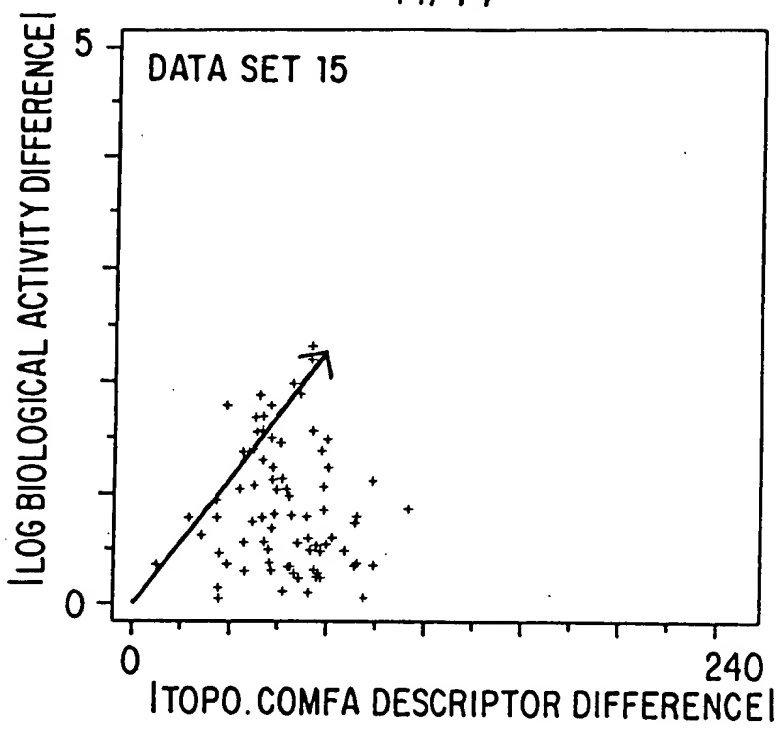


FIG.7(o)

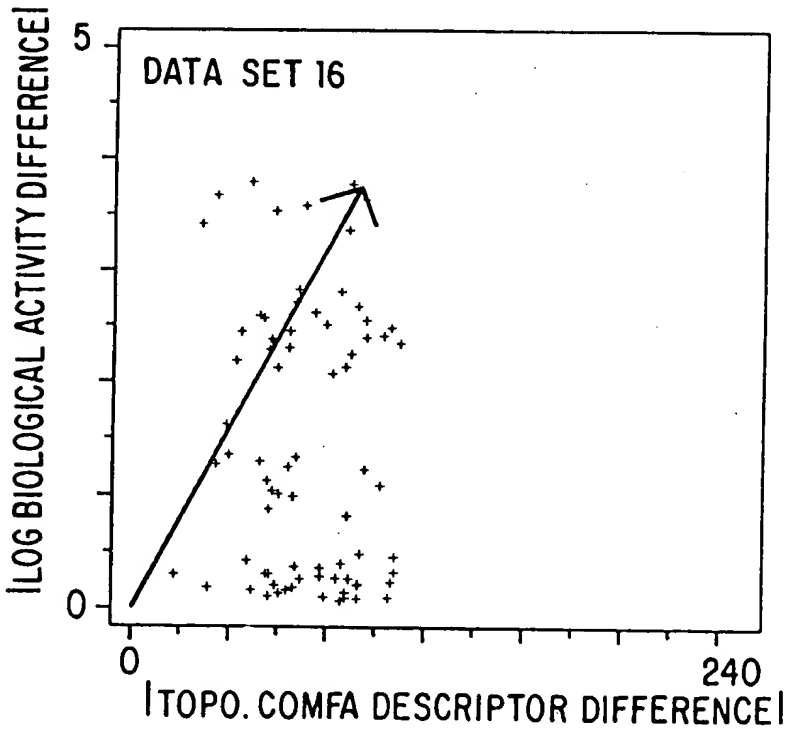


FIG.7(p)

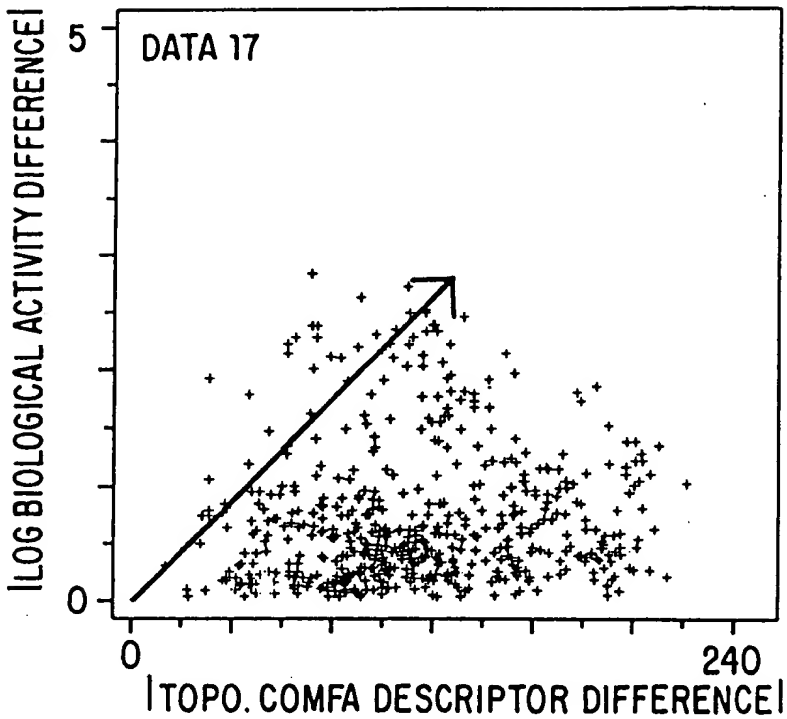

DATA 17
5
0
0
240
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG.7(q)

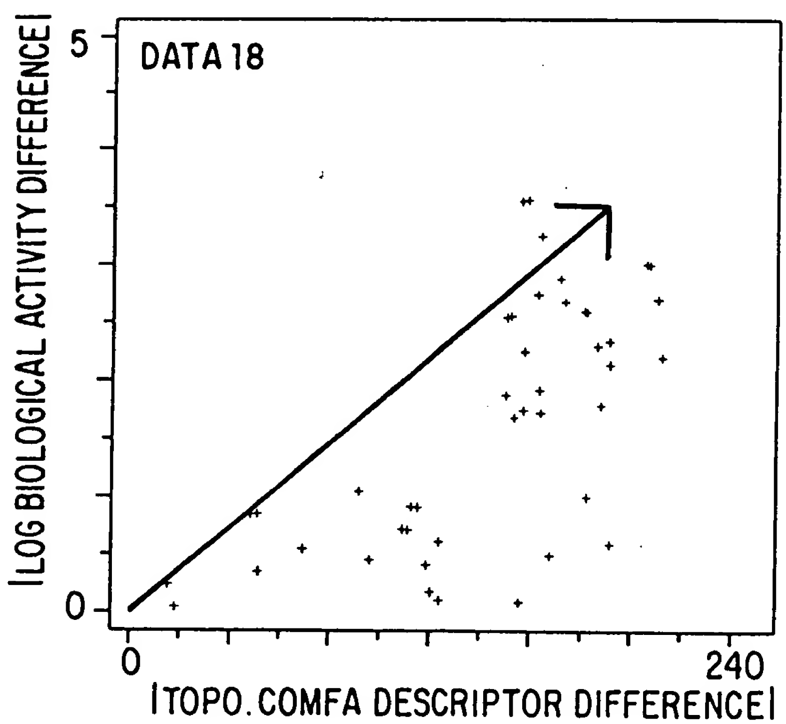

DATA 18
5
0
0
240
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG.7(r)

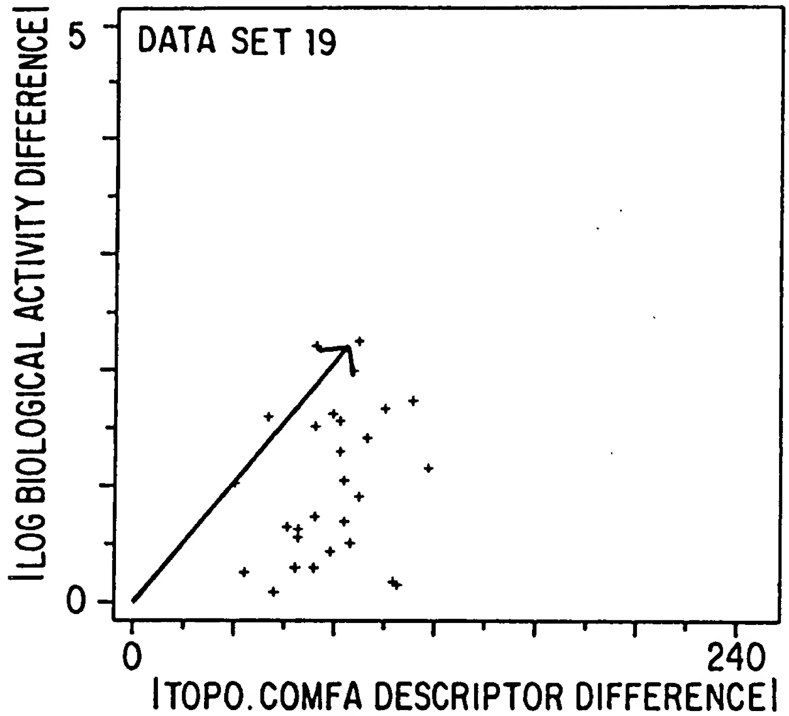

DATA SET 19
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
5
0
0
240
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG. 7(s)

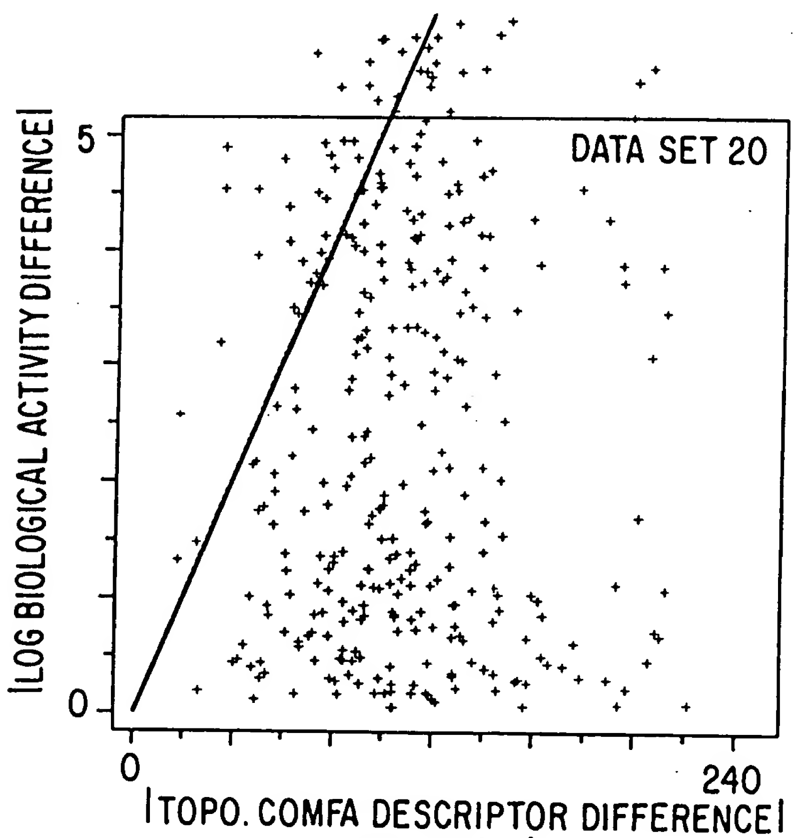

DATA SET 20
|LOG BIOLOGICAL ACTIVITY DIFFERENCE|
5
0
0
240
|TOPO. COMFA DESCRIPTOR DIFFERENCE|

FIG. 7(t)

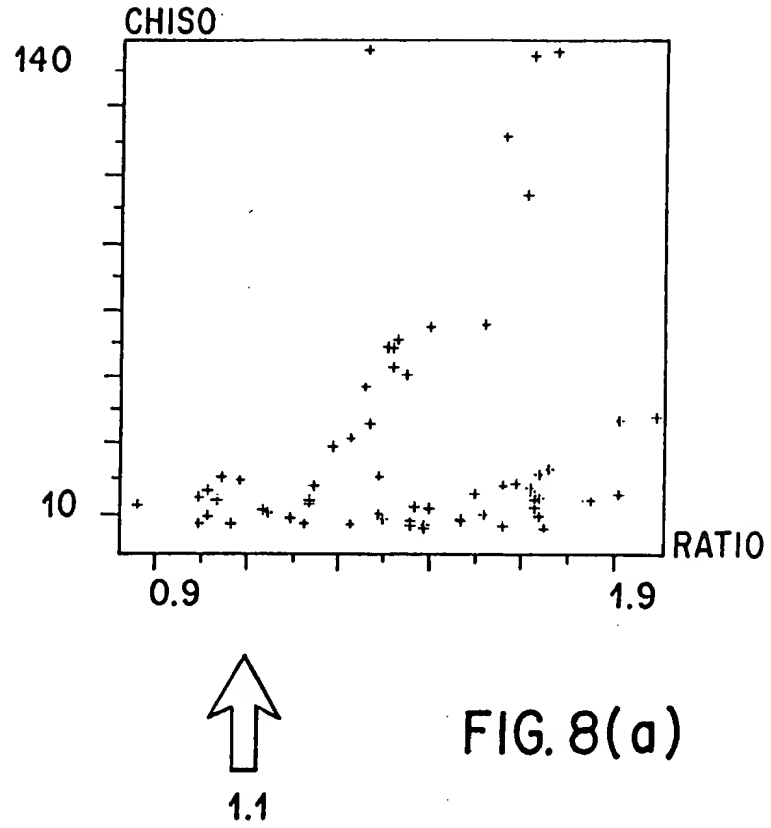


FIG. 8(a)

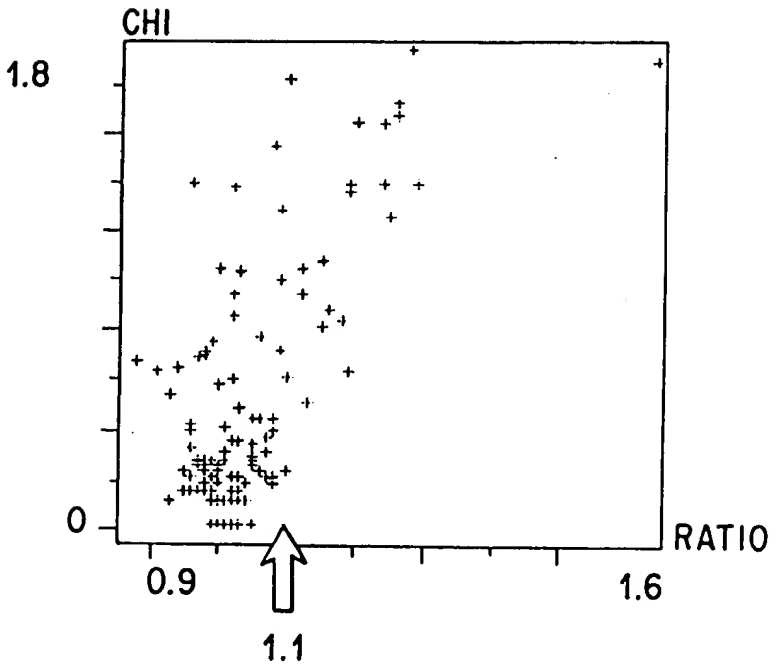


FIG. 8(b)

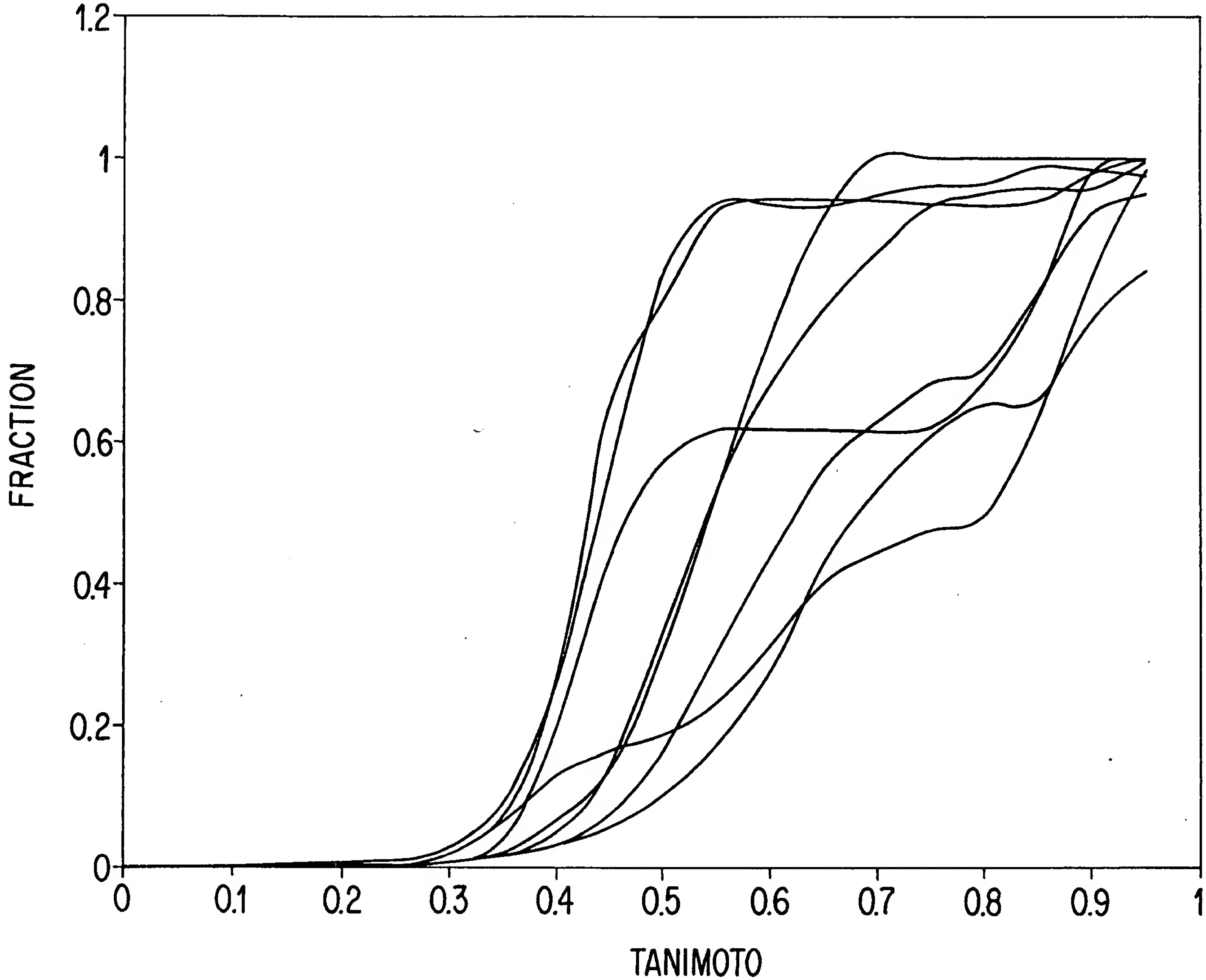


FIG. 9(a)

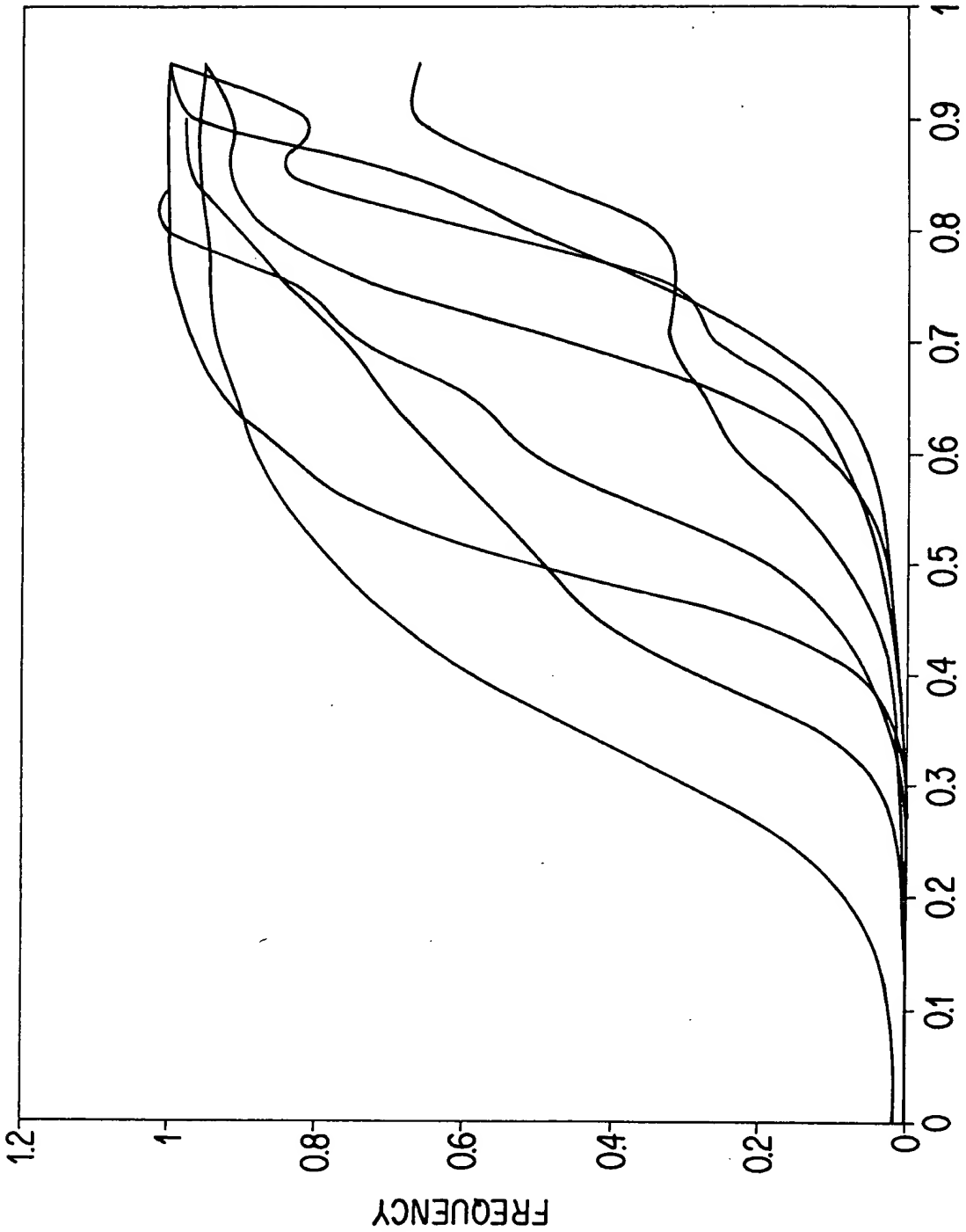


FIG. 9(b)

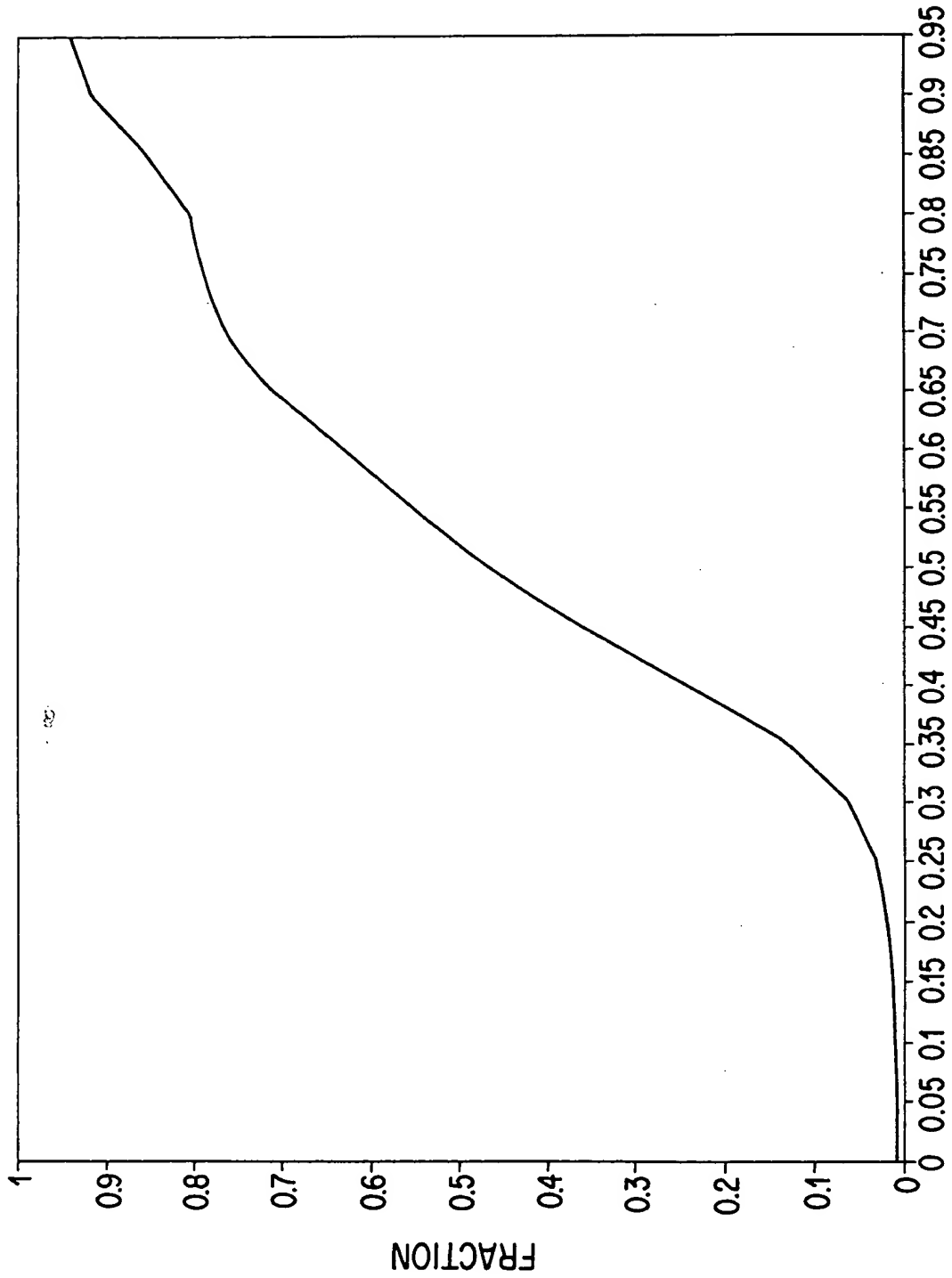

FRACTION
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95
TANIMOTO

FIG. 9(c)

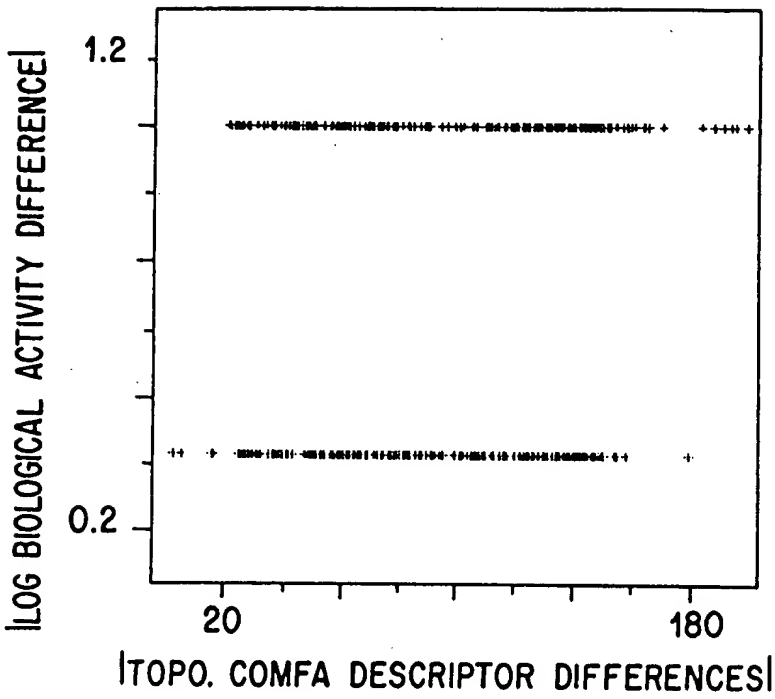


FIG. 10(a)

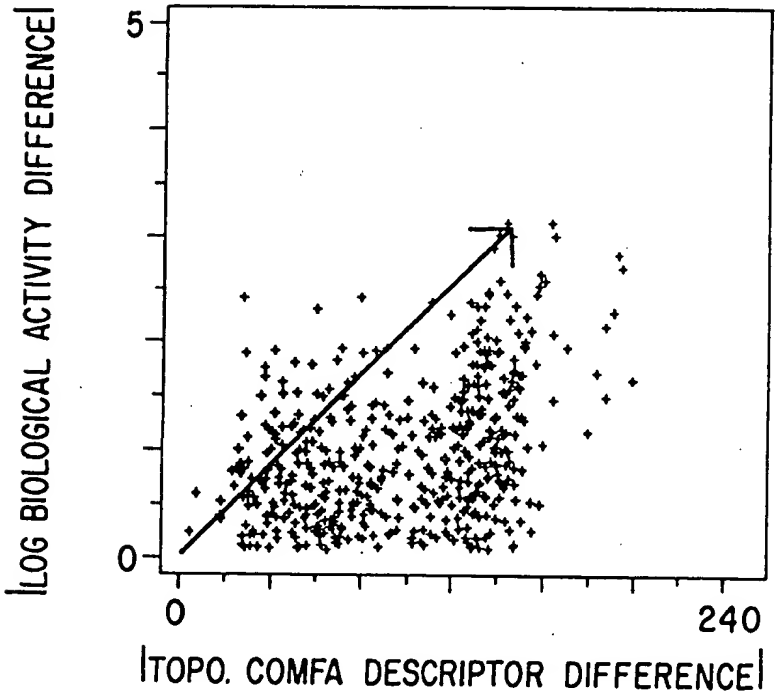


FIG. 10(b)

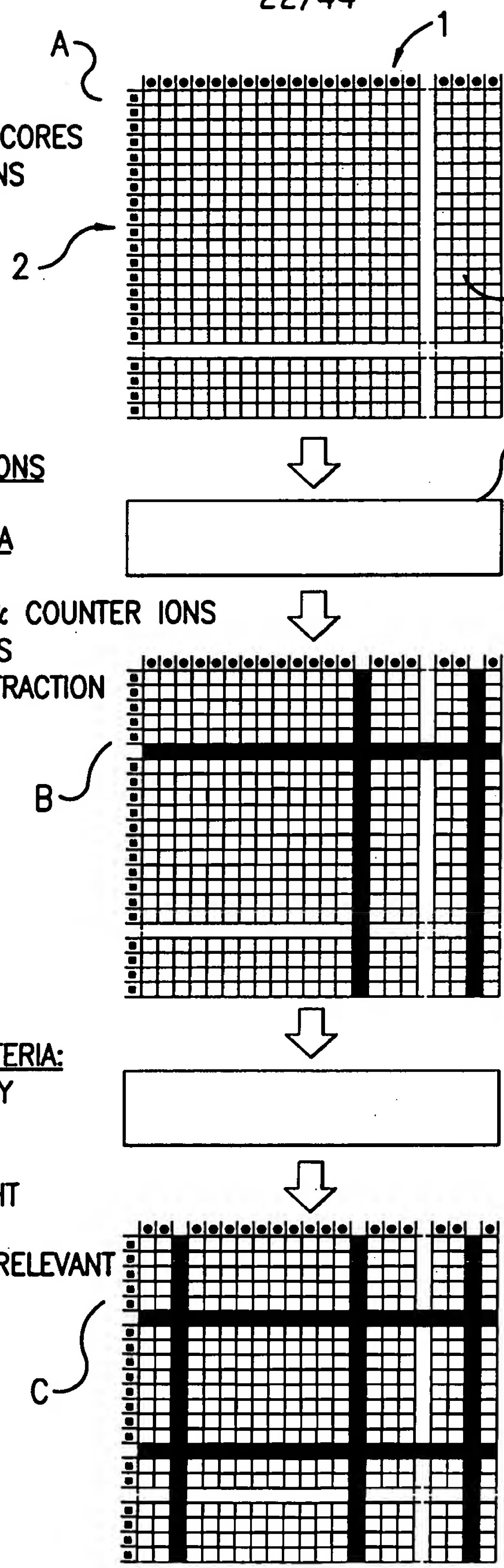
FUNCTION

8.
SELECT CHEMISTRY
LIST REACTANTS & CORES
DEFINE COMBINATIONS

8.A
REMOVE REACTANTS:
NON-DIVERSITY REASONS

8A(i) GENERAL CRITERIA
METALS
TAUTOMERS/SALTS & COUNTER IONS
INTERFERING GROUPS
SYNTHESIS & EXTRACTION
PRICE/AVAILABILITY

8.(A)ii BIOLOGICAL CRITERIA:
TOXIC/METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP
NON-BIOLOGICALLY RELEVANT GROUPS
SUGARS/MULTIPLE FUNCTIONALITIES



SOFTWARE

ANY DATABASE OR WORD PROCESSING PROGRAM

ANY WORD PROCESSING PROGRAM OR MOLECULAR SPREAD SHEET (MSS)

SYBYL: SPL SCRIPTS ON MSS INVOKING-UNITY SEARCHES FOR FRAGMENTS CALCULATIONS OF MW & CLOGP

FIG.11(a)

8B

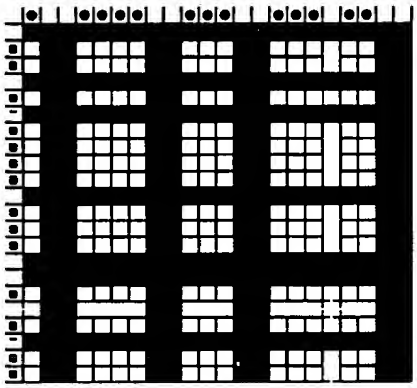
REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
TOPOMERIC CONFORMER ALIGNMENT
CoMFA FIELD GENERATION:
HYDROGEN BOND FIELD GENERATION
ROTATABLE BOND FIELD ATTENUATION
CALCULATE FIELD DIFFERENCES
CLUSTER
REACTANT SELECTION FROM EACH CLUSTER

D

SYBYL: SELECTOR & CONCORD 3.2.1 SPECIALIZED SOFTWARE: APPENDIX "A" (SYBYL: CoMFA STERIC & MSS)

SYBYL: HIERCHICAL CLUSTER - MSS
SYLBL: MSS

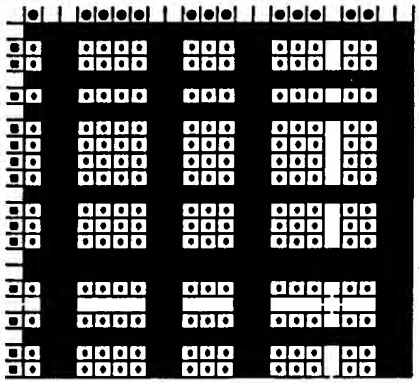


8C

COMBINE REACTANTS TO BUILD PRODUCTS

SYBYL: LEGION MSS

E



8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:

SYBYL: SPL SCRIPTS ON MSS

F

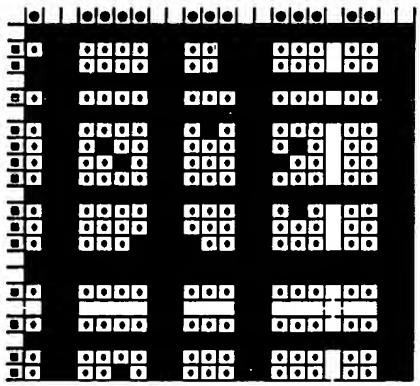
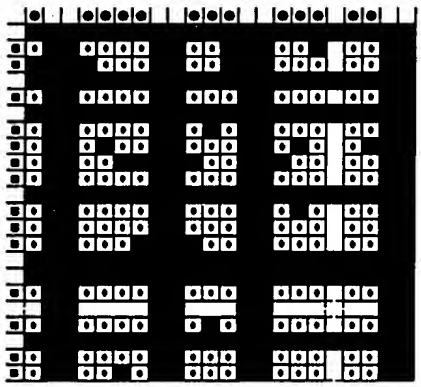


FIG.11(b)

8D
BIOLOGICAL CRITERIA:
METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP

SYBYL: SPL SCRIPTS ON MSS INVOKING –
UNITY SEARCHES FOR FRAGMENTS
CALCULATIONS OF MW & CLOGP

G



8E
REMOVE NON-DIVERSE PRODUCTS:

GENERATE TANIMOTO 2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN $\geq$ 0.85

UNITY

H

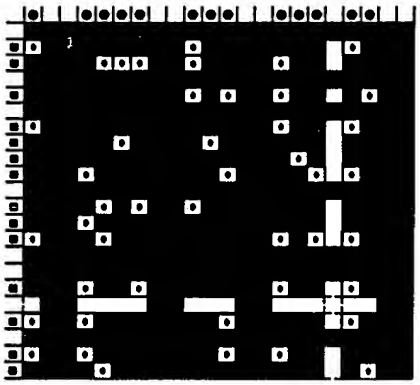


FIG.11(c)

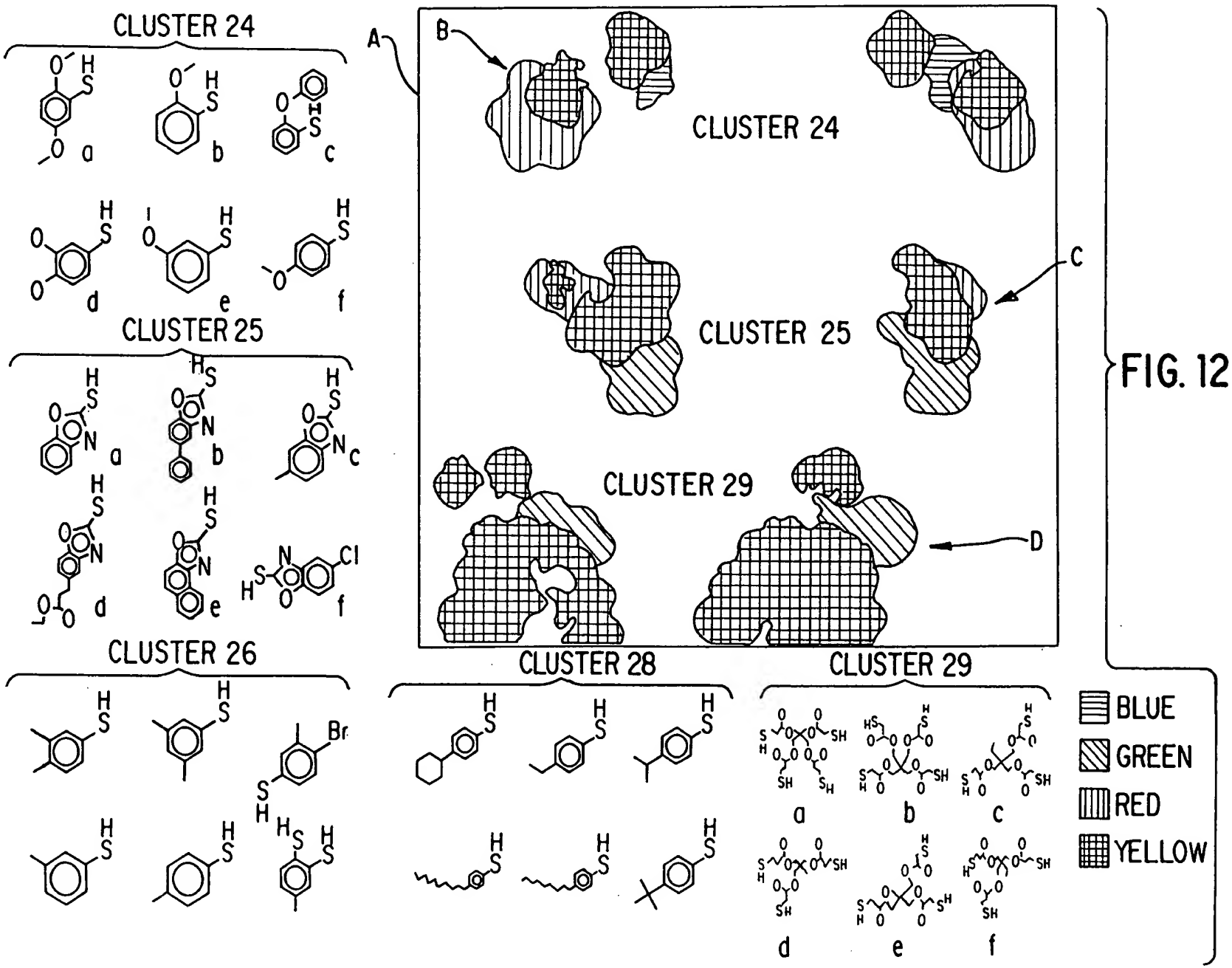

CLUSTER 24
a
b
c
d
e
f
CLUSTER 25
a
b
c
d
e
f
CLUSTER 26
A
B
CLUSTER 24
CLUSTER 25
C
CLUSTER 29
D
CLUSTER 28
CLUSTER 29
a
b
c
d
e
f
BLUE
GREEN
RED
YELLOW

FIG. 12

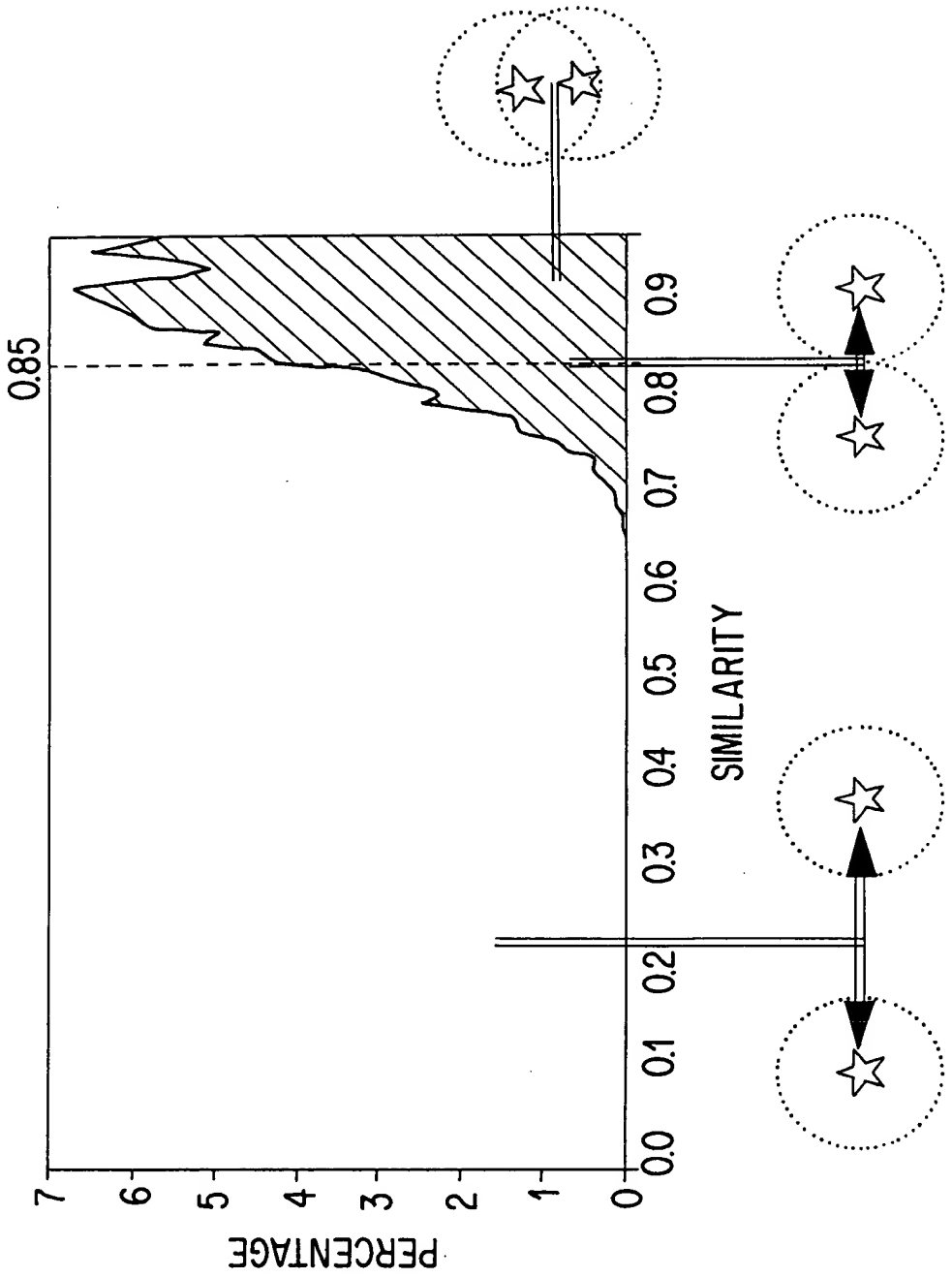


FIG. 13

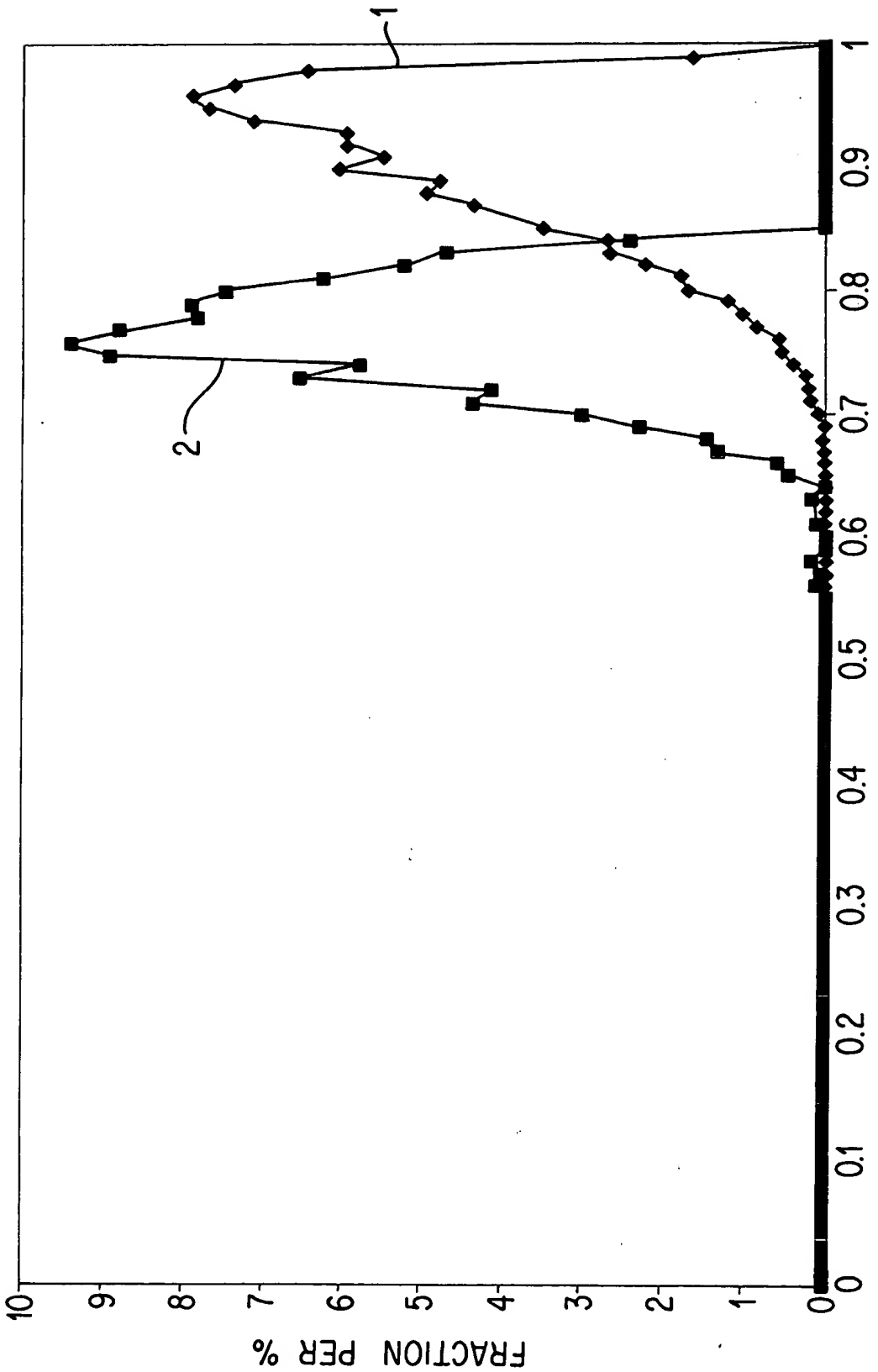


FIG.14

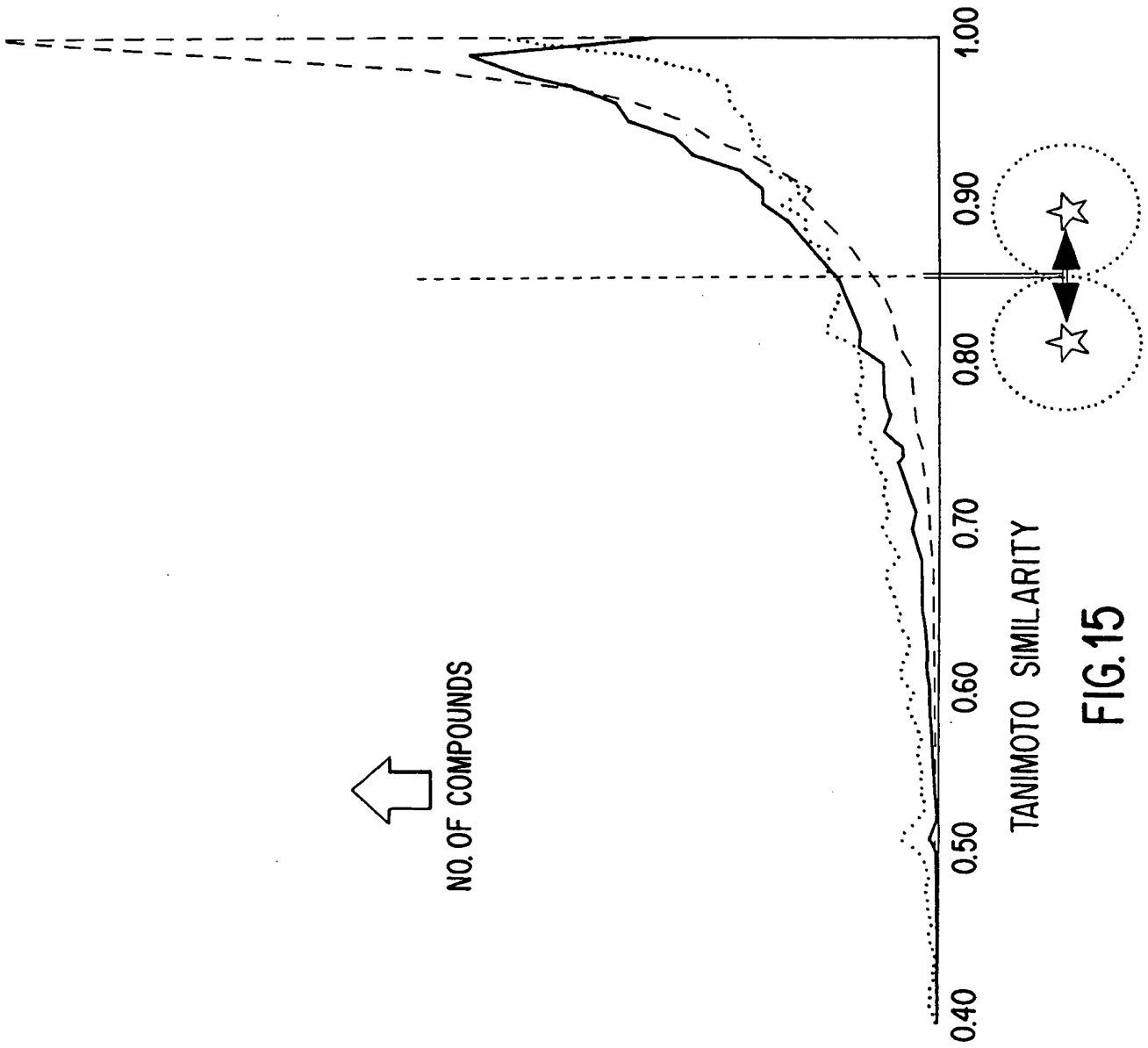


FIG.15

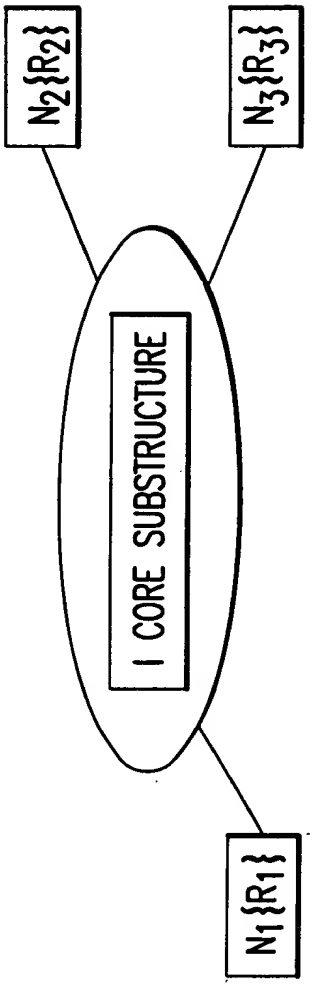


FIG.16

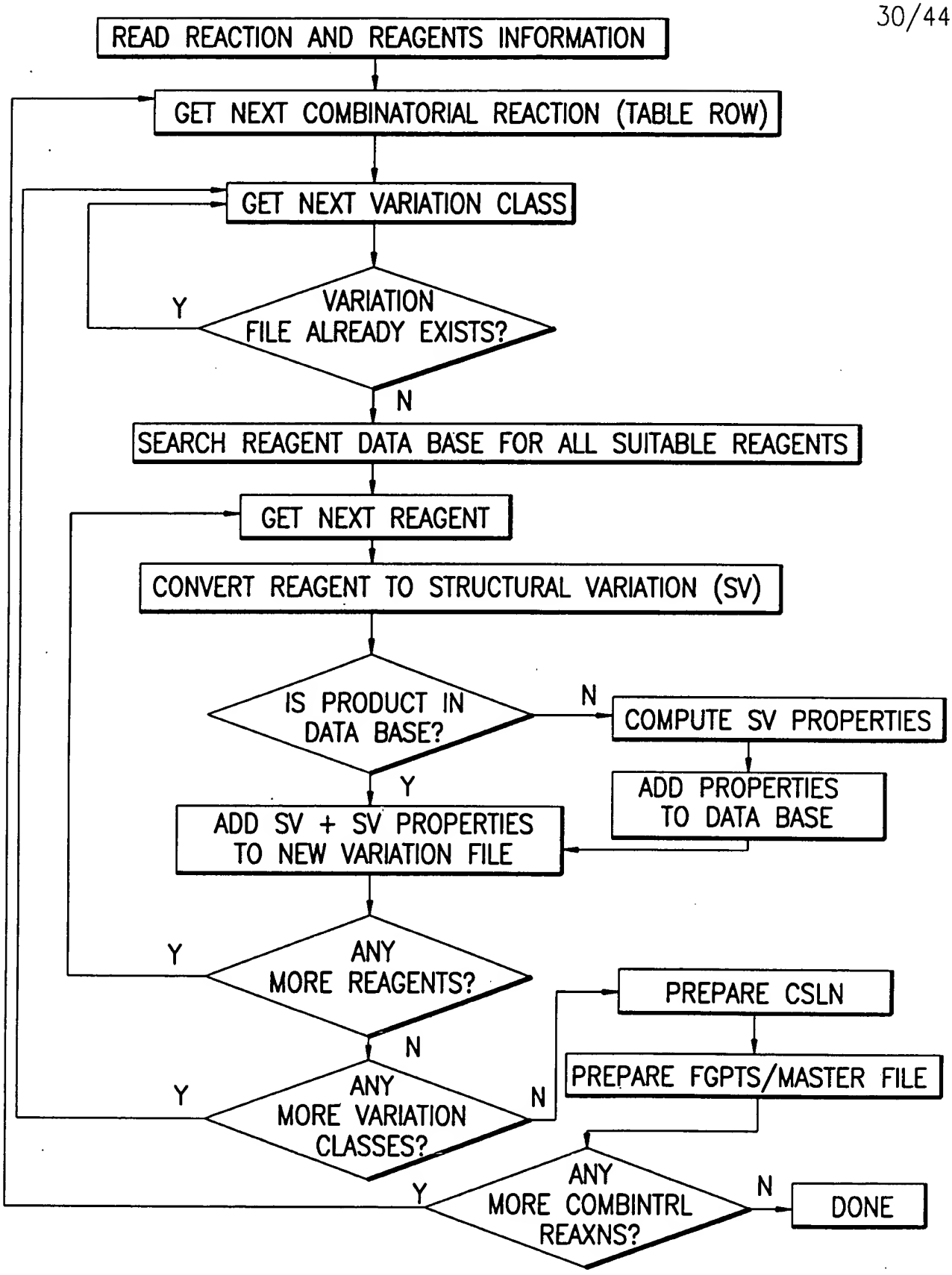


FIG.17

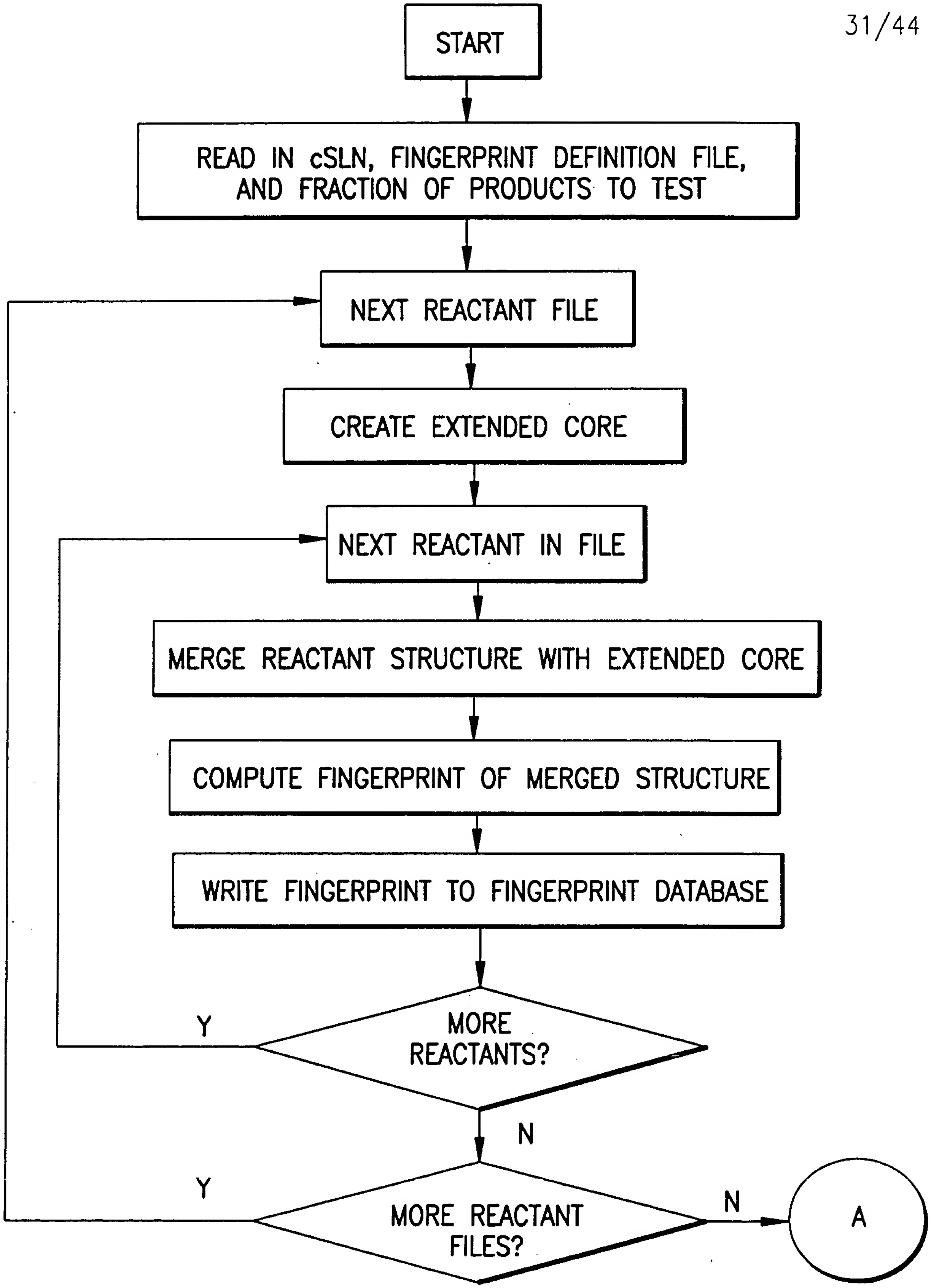


FIG.18

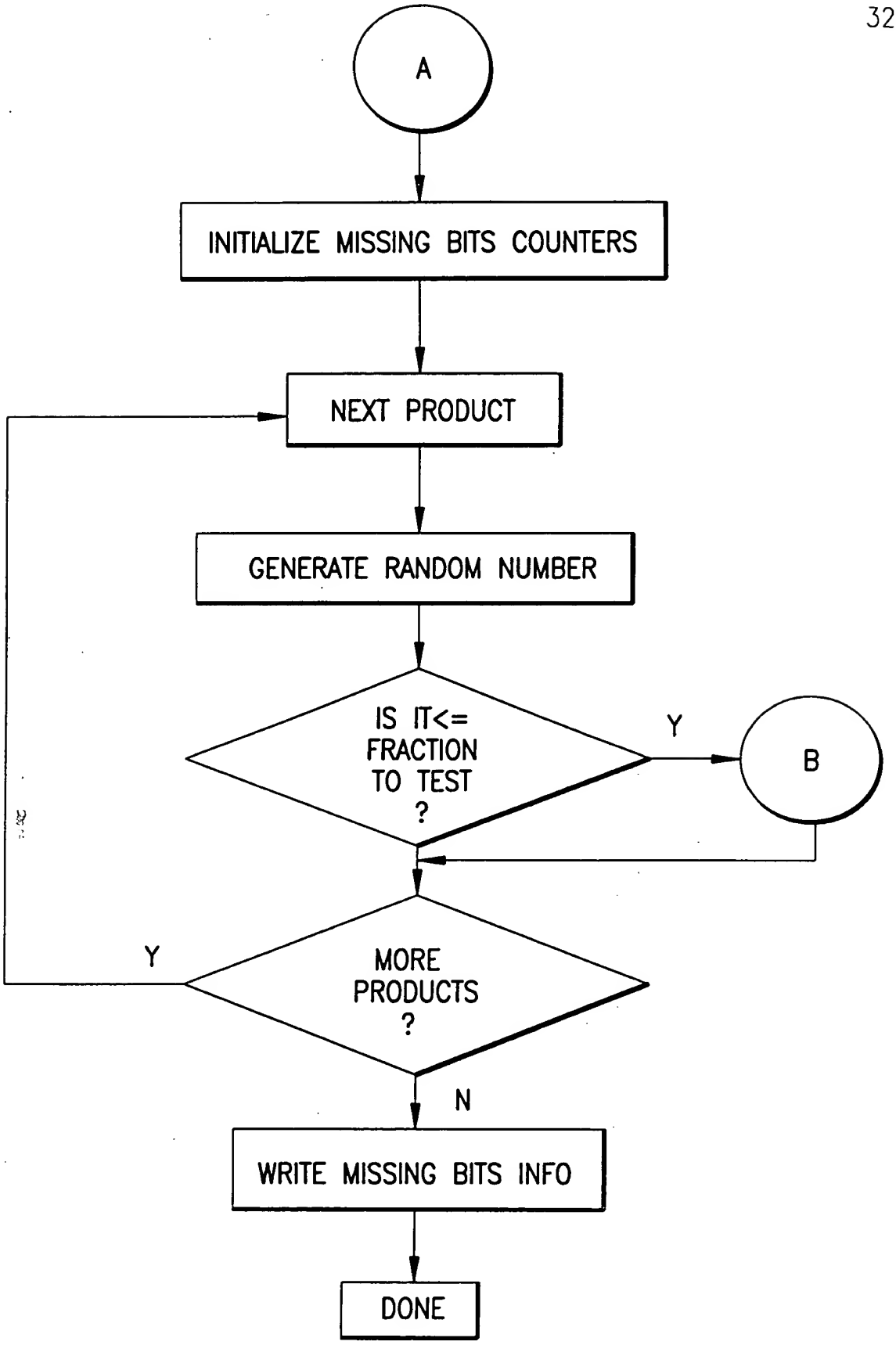


FIG.19

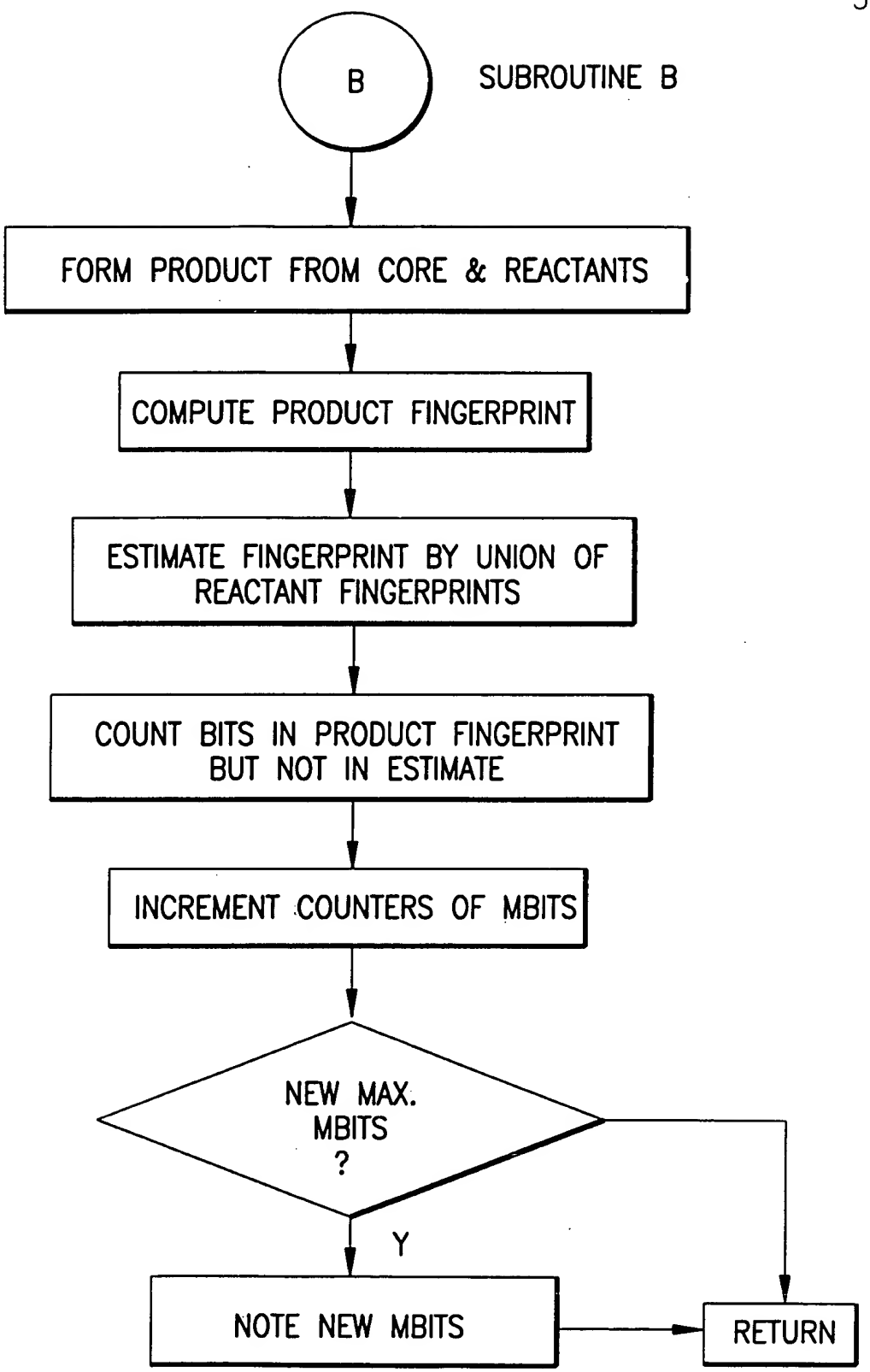


FIG.20

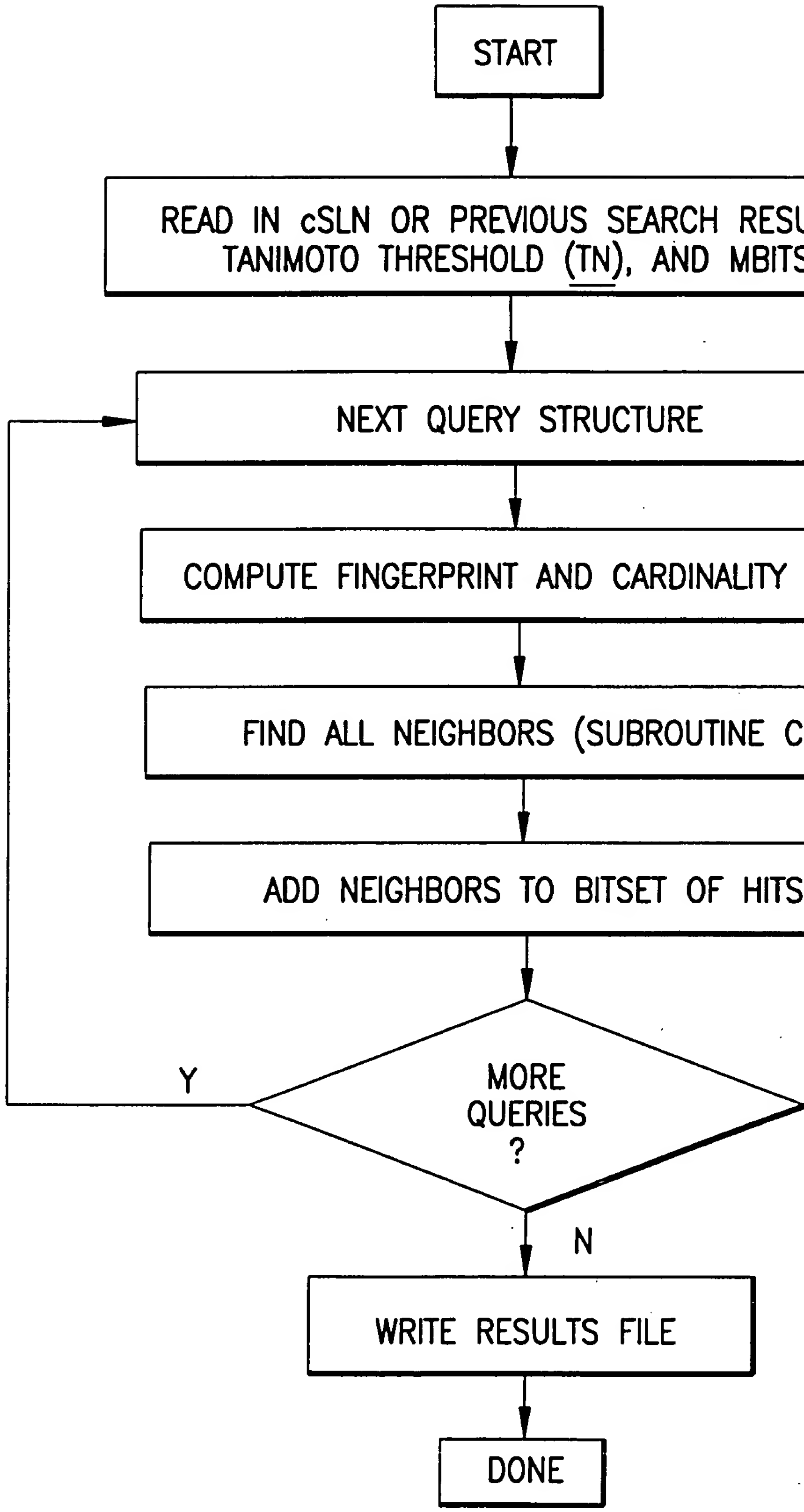


FIG.21

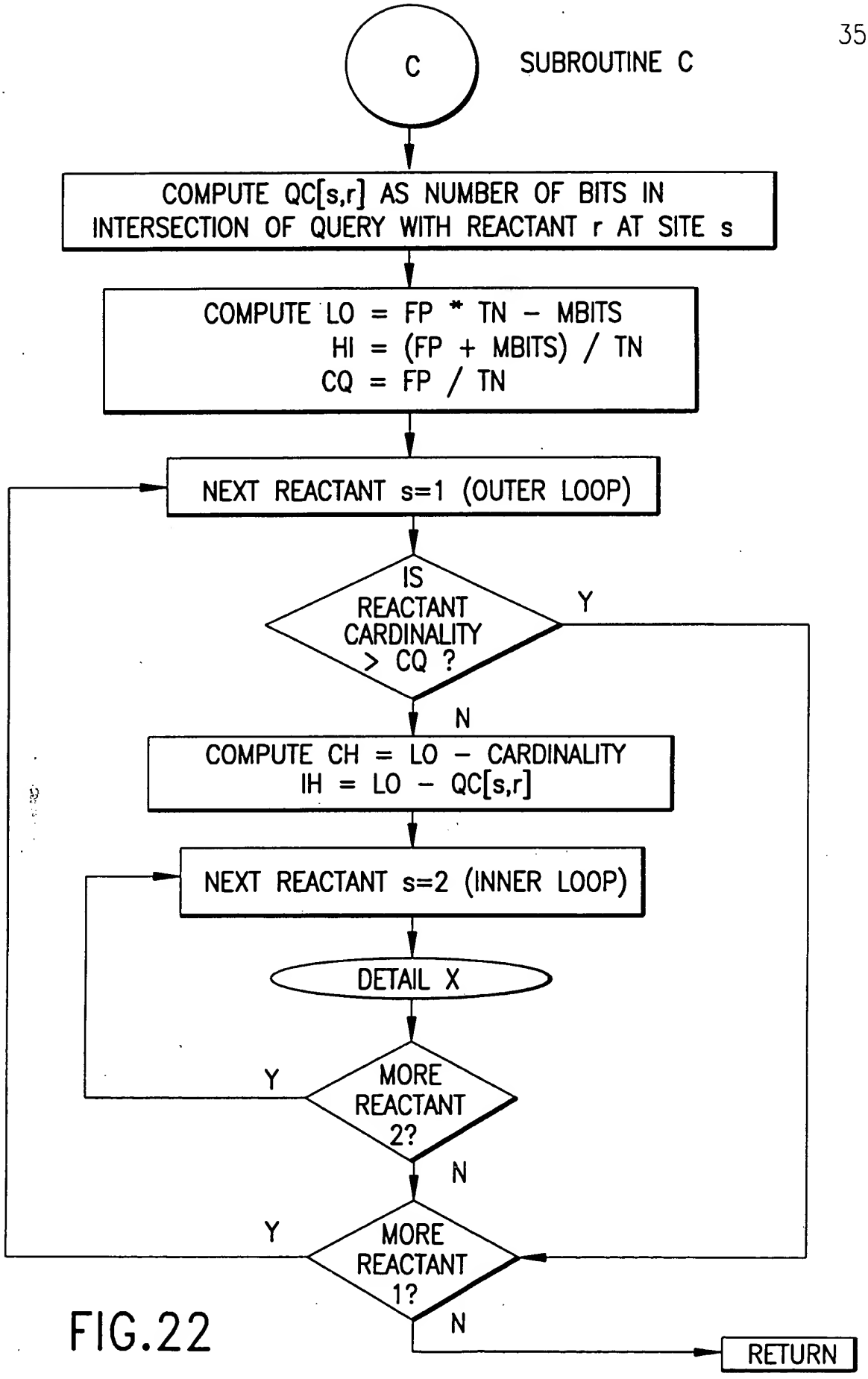


FIG.22

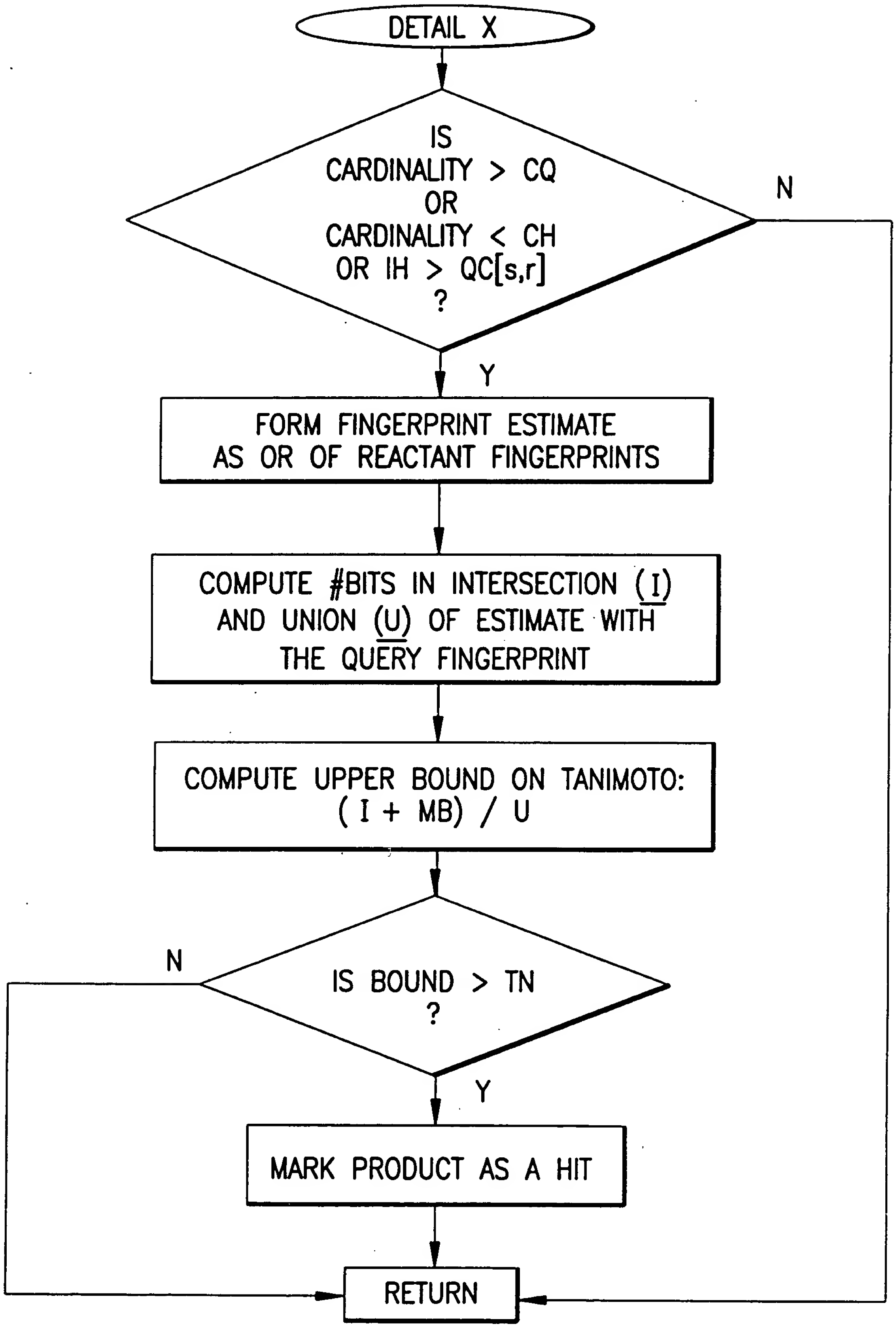


FIG.23

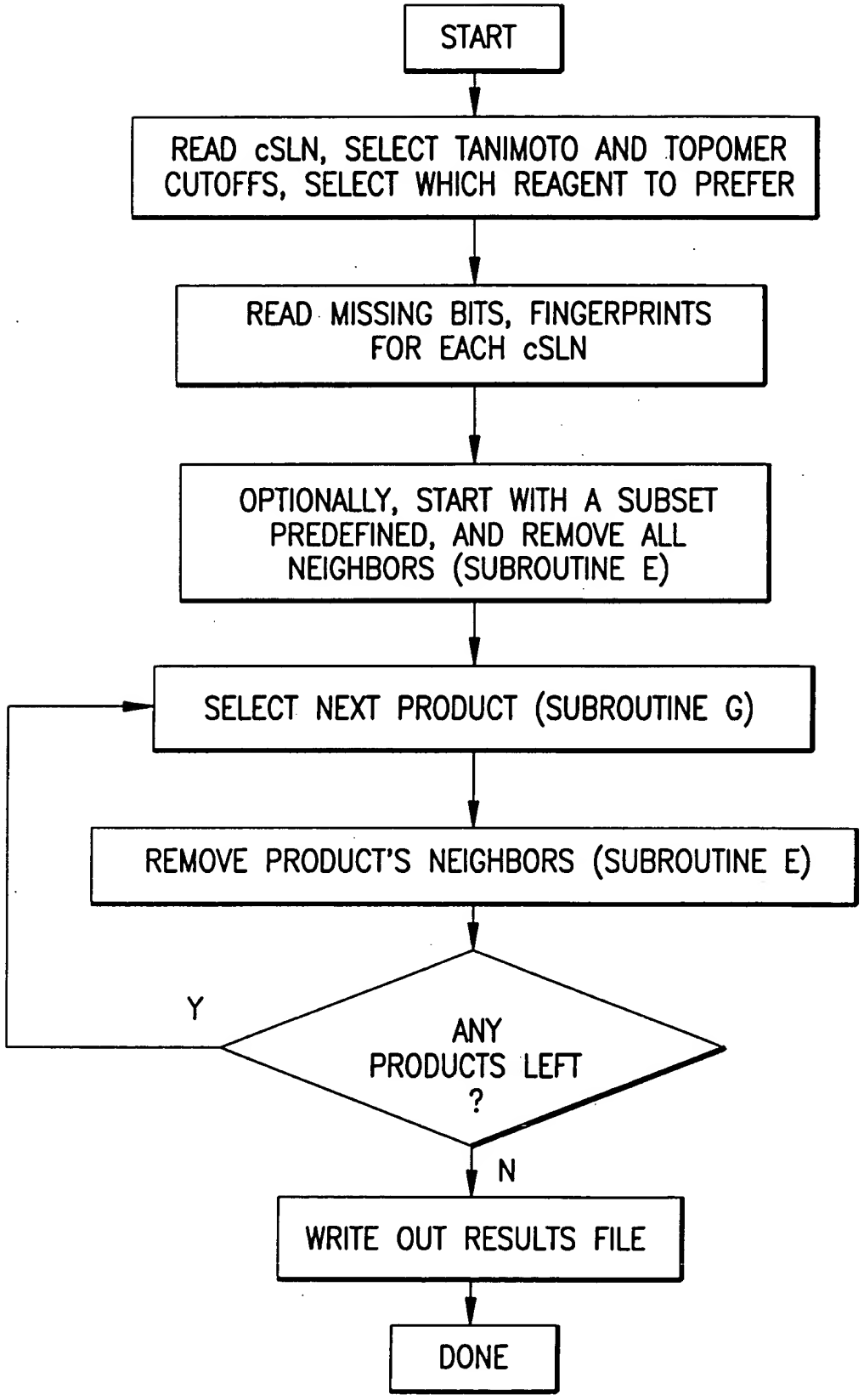


FIG.24

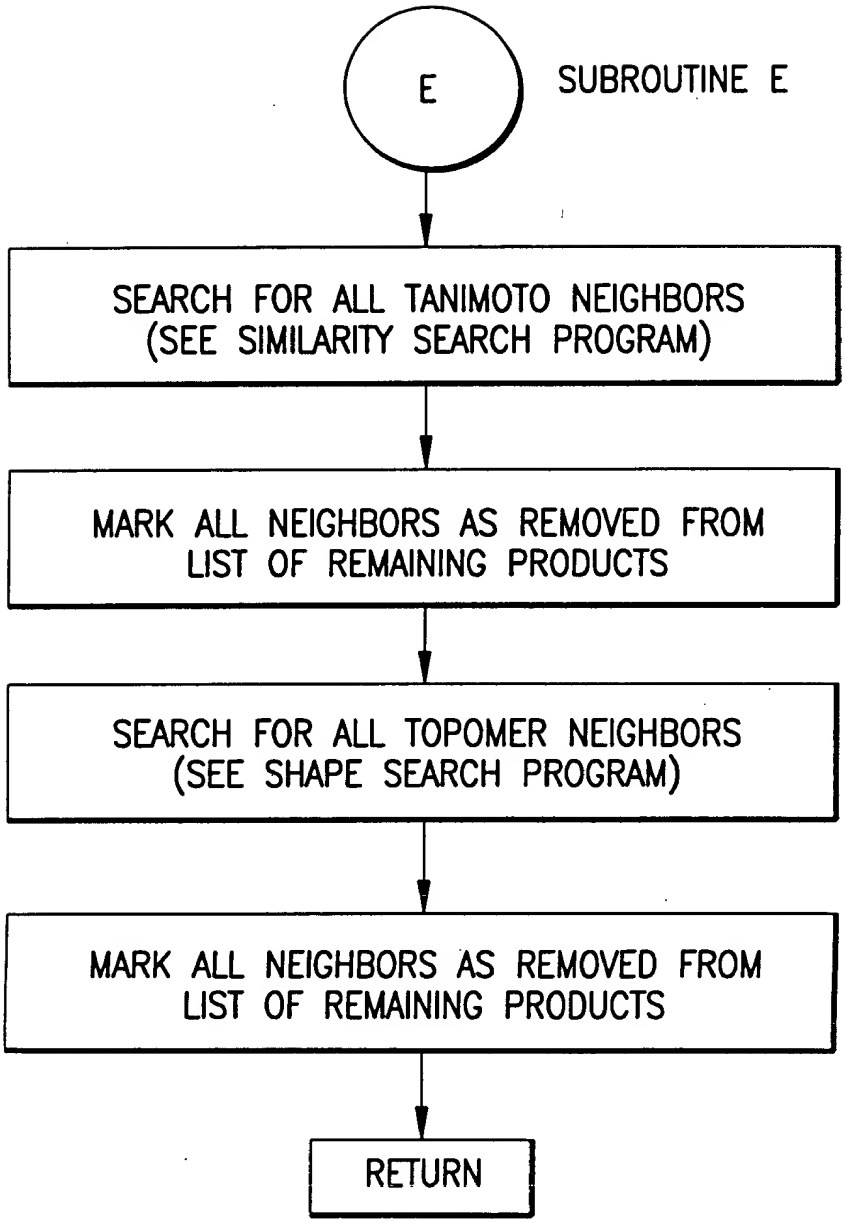


FIG.25

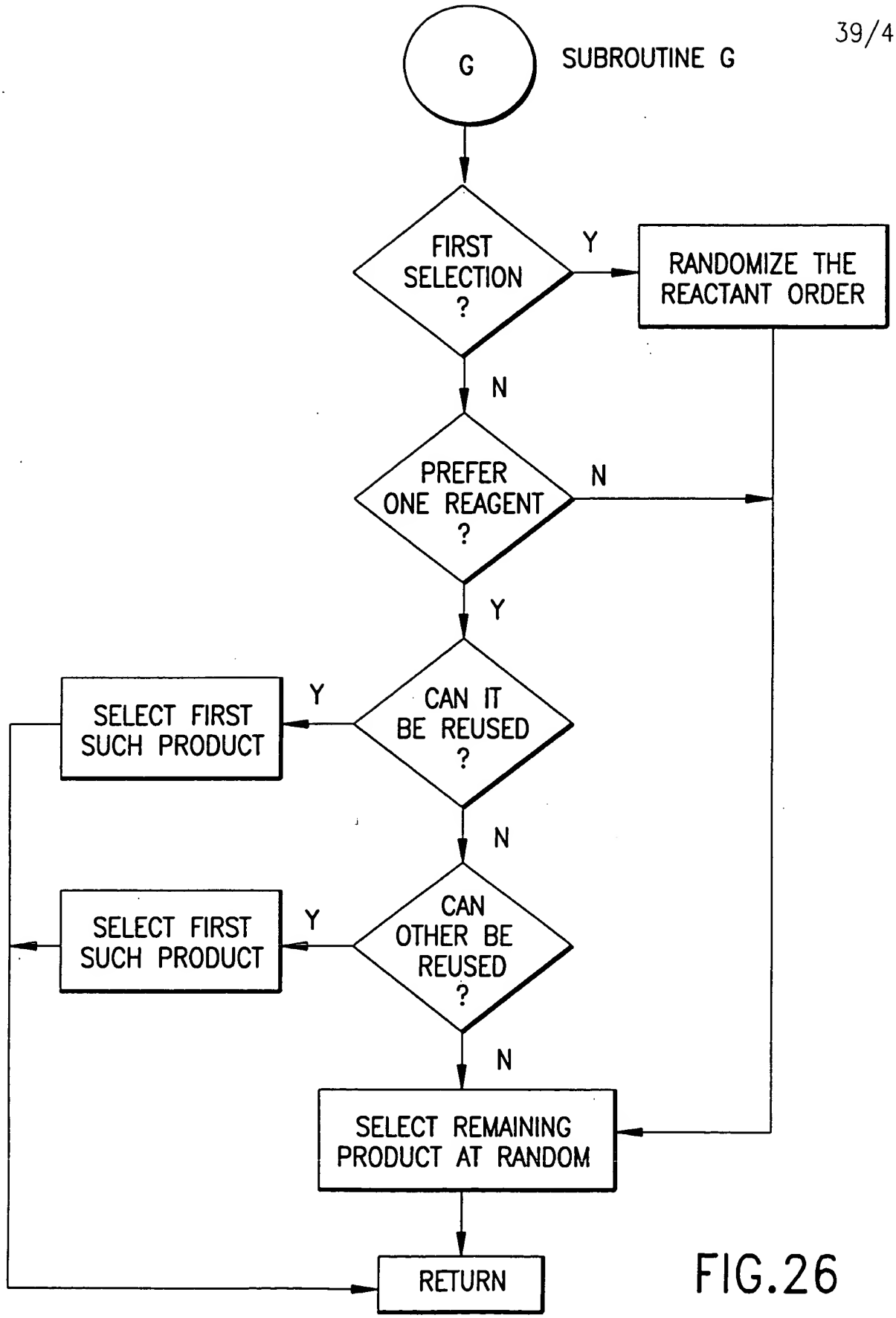


FIG.26

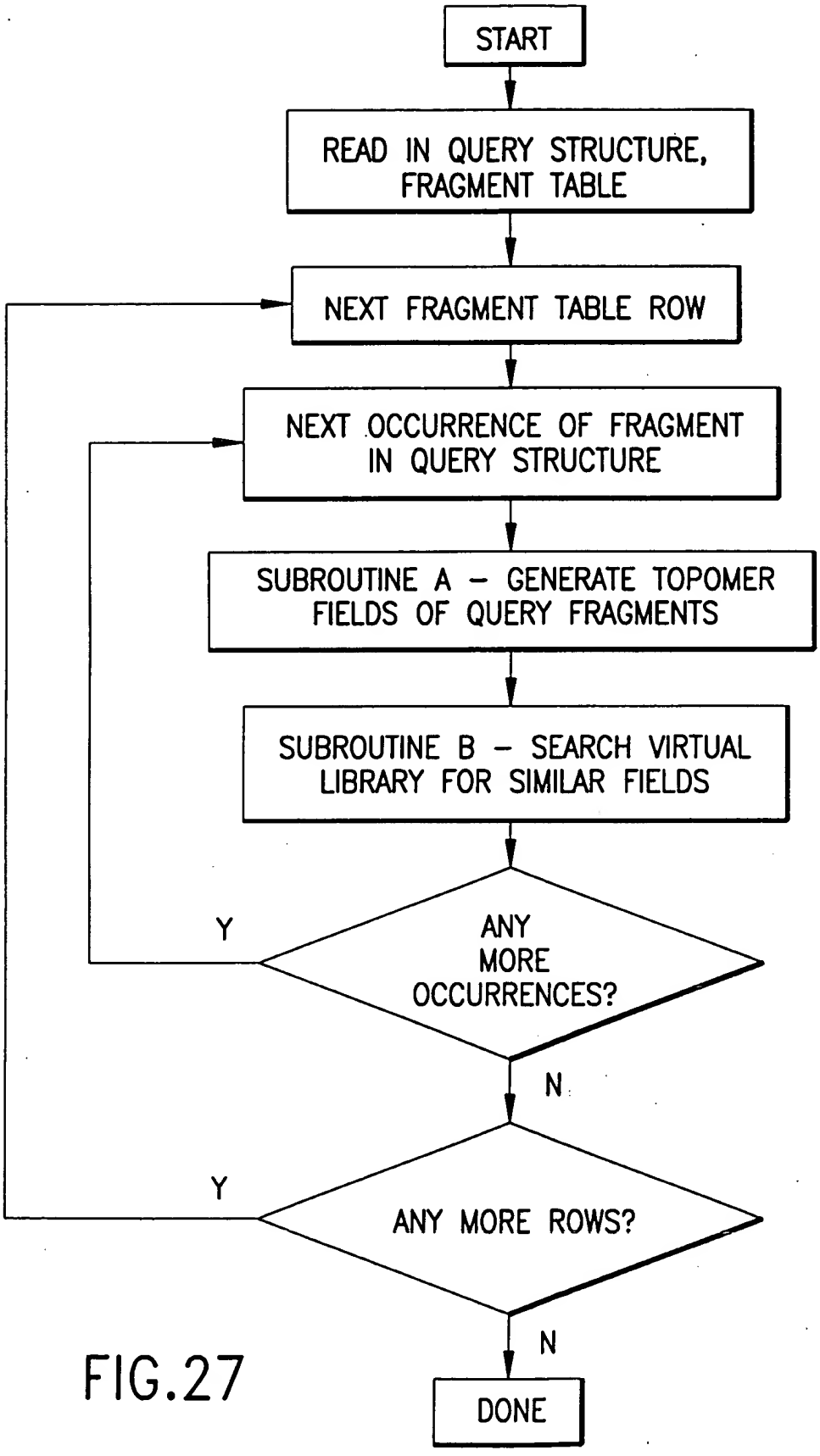


FIG.27

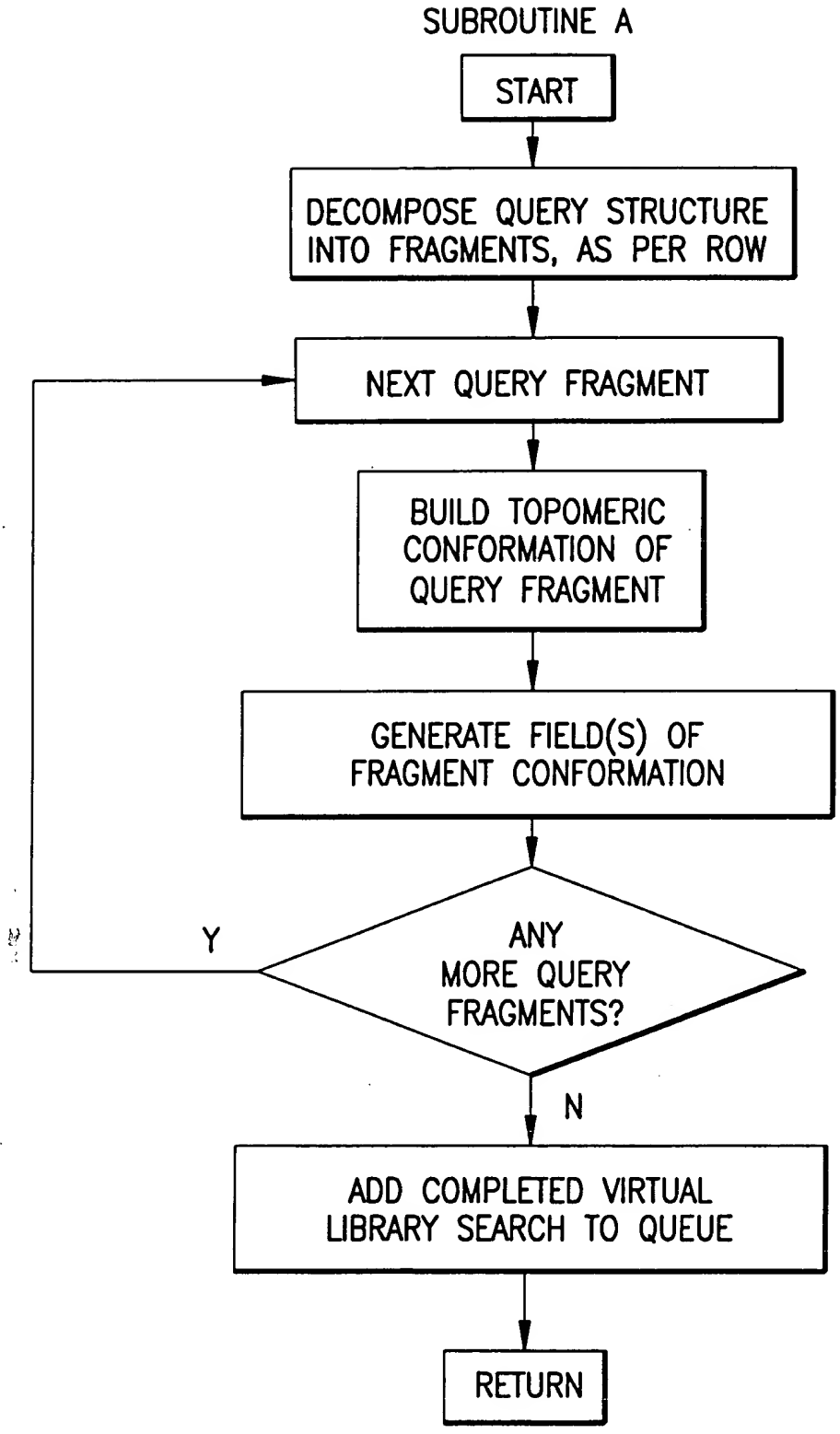


FIG.28

SUBROUTINE B

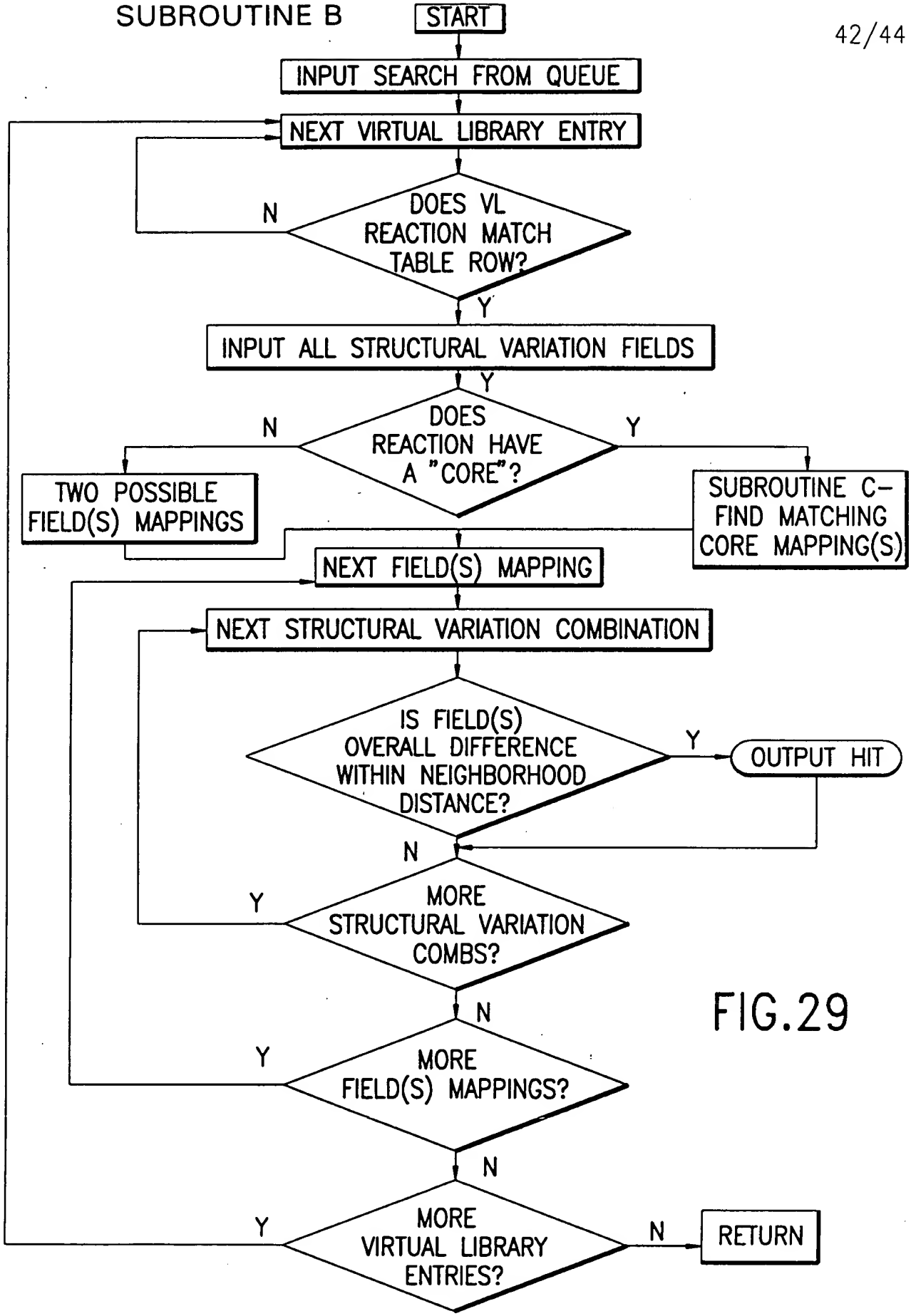


FIG.29

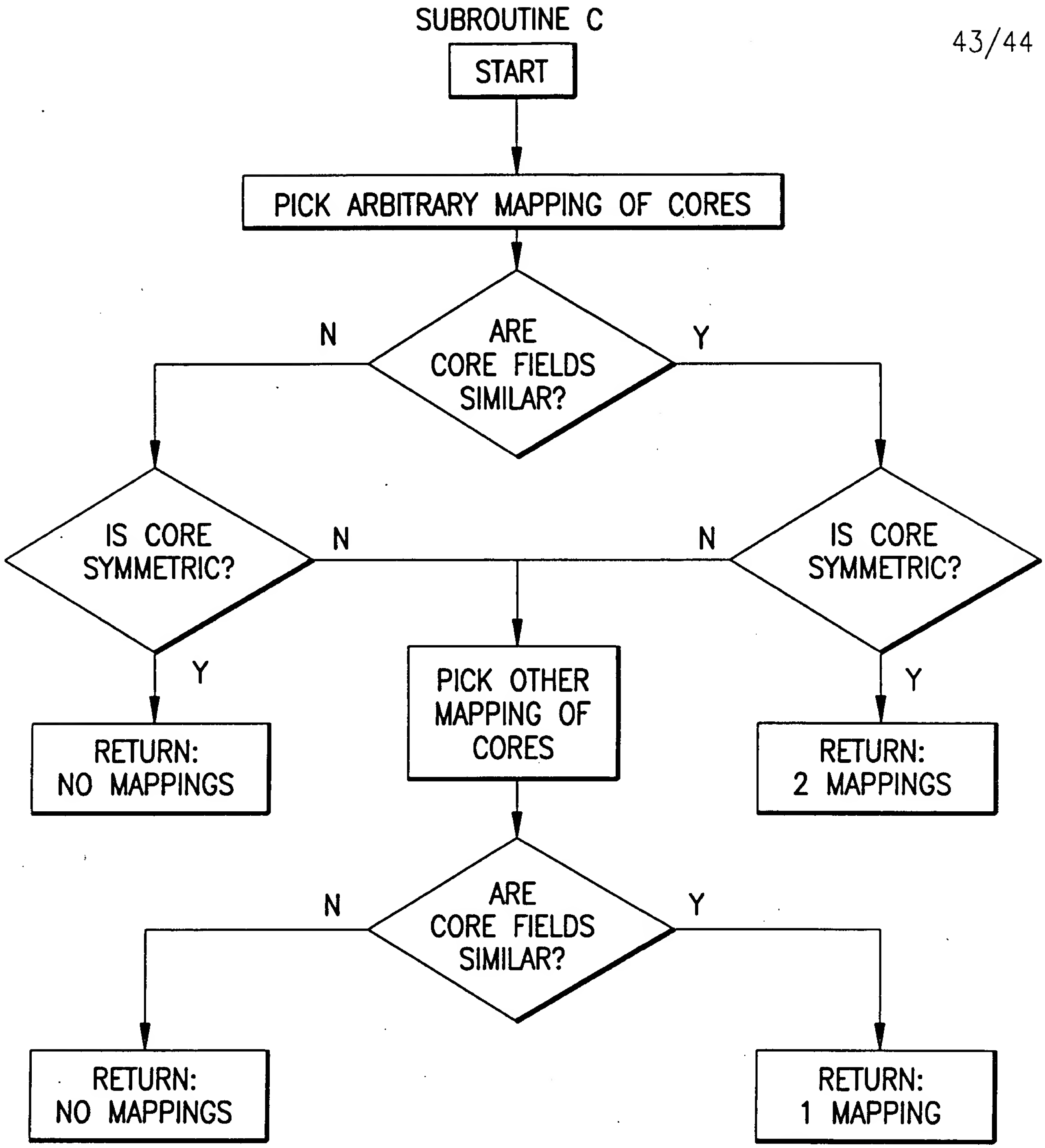


FIG.30

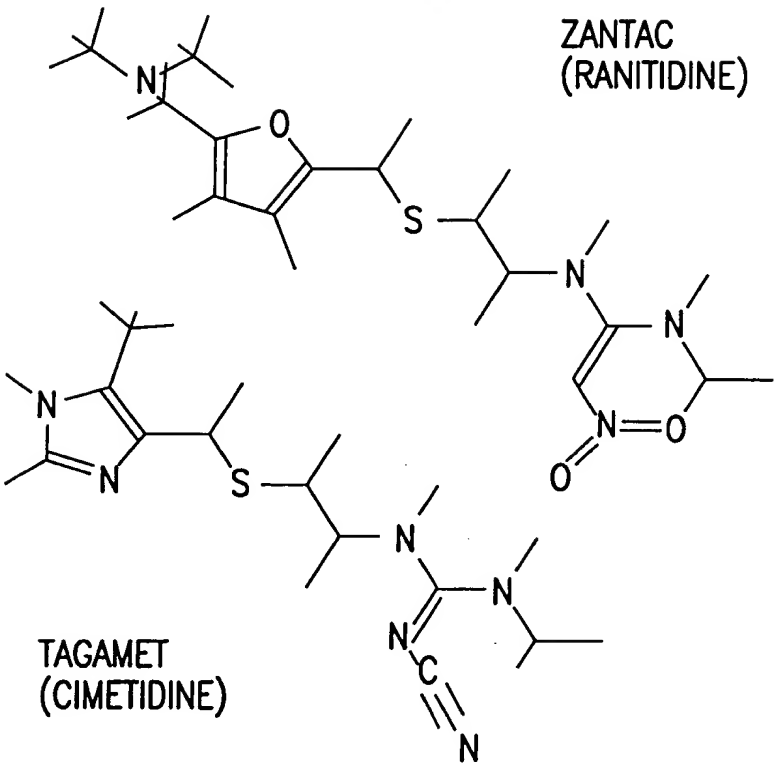


FIG.31